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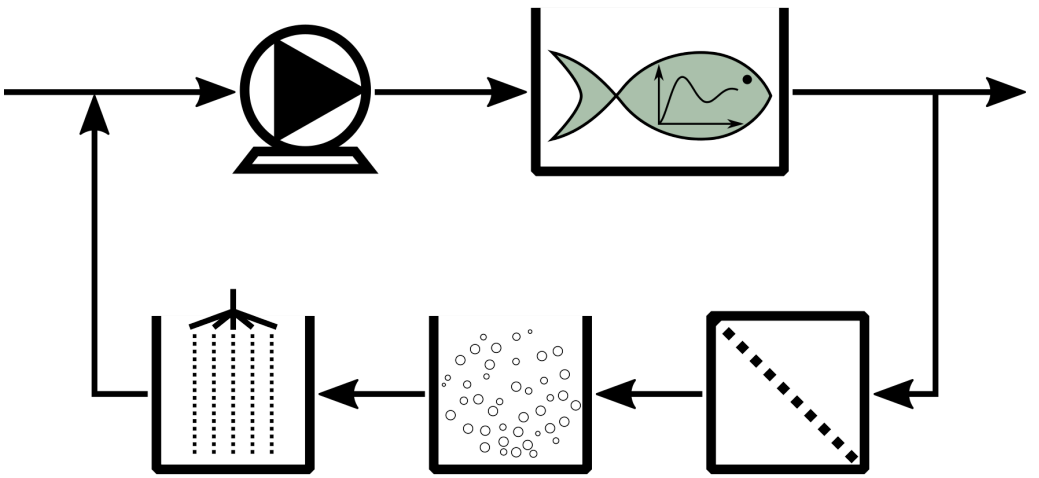

Simulation and Optimization of Recirculating Aquaculture Systems

SIMON PEDERSEN

Department of Electrical Engineering
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden, 2018

THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

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Simon Pedersen

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Technical Report No. R010/2018
ISSN 1403-266X
This thesis has been prepared using LaTeX.

Department of Electrical Engineering
Chalmers University of Technology
SE-412 96 Göteborg, Sweden
Phone: +46 (0)31 772 1000
www.chalmers.se

Printed by Chalmers Reproservice
Göteborg, Sweden, October 2018

Abstract

Recirculating aquaculture – intensive fish farming with water treatment and reuse – has great potential as a method for sustainable food production. Benefits over traditional aquaculture include opportunities to reduce nitrogen emissions to water, control of temperature, salinity and pH, reduced environmental impact of escapes and better protection against e.g. parasites and pathogens. Building a water treatment system is however a significant investment, which makes the optimality of the design important. Unfortunately, the biological nature of these plants leads to incredibly slow dynamics, which makes experimental development very tedious and expensive.

Water treatment in recirculating aquaculture systems (RAS) typically consist of particle removal (settling and/or filtering), degassing of carbon dioxide, biological removal of organics and nitrogenous waste, oxygenation of water and (optionally) application of ozone or UV against pathogens. Dimensioning the various units is often done using steady state mass balances that do not capture the complex interactions present in biological water treatment systems. Simulations of integrated dynamical models of fish growth, waste production and water treatment have previously been shown to be useful in exploring these interactions, and with enough fidelity, computer models can greatly improve the speed at which recirculating aquaculture can be developed.

In this thesis, a framework for dynamical modelling of recirculating aquaculture systems is presented. It is based on the well-established Activated Sludge Model no. 1 together with models of fish growth, feeding, digestion and evacuation. The model has been implemented in Modelica to produce a dynamic RAS simulator that is the successor to FishSim, with greatly improved performance and robustness. A genetic optimization routine was used with the simulator in order to investigate the impact of different layouts, or topologies, on the performance of the water treatment in a RAS.

Three different water treatment topologies, two fish species (Rainbow trout and Atlantic salmon), two influent oxygen saturation levels and both semi-closed and fully recirculating versions were compared, for a total of 24 cases. Each case was optimized in terms of required biofilter volume to maintain an acceptable total ammonia nitrogen (TAN) concentration in the fish tank. The results indicate that the smallest volume is obtained by introducing several bypass flows in the treatment system of a semi-closed RAS. In a fully closed system with minimal water exchange, denitrification is required to prevent excessive accumulation of nitrate, and then the flows of oxygen, carbon and nitrogen must be carefully considered. For several of the cases, no optimum with denitrification could be found.

We conclude that no overall best configuration and operation strategy for water treatment could be found, but rather that it varies depending on the conditions imposed by the fish culture. This highlights how simulations can be an important tool in gaining understanding about the behaviour of recirculating aquaculture systems.

Keywords: Recirculating aquaculture, dynamic modelling, wastewater treatment

Acronyms

AOB:	Ammonia oxidizing bacteria
ASM:	Activated sludge model
BOD:	Biological oxygen demand
COD:	Chemical oxygen demand
CSBR:	Continuous stirred biofilm reactor
CSTR:	Continuous stirred tank reactor
DN:	Denitrification
DO:	Dissolved oxygen
FCR:	Feed conversion ratio
HRT:	Hydraulic retention time, V/Q
IBW:	Initial body weight
MBBR:	Moving bed biofilm reactor
NOB:	Nitrite oxidizing bacteria
RAS:	Recirculating aquaculture system(s)
TAN:	Total ammonia nitrogen
TGC:	Thermal growth coefficient
TOC:	Total organic carbon
PI:	Proportional-integrating (controller)

Mathematical symbols

Lowercase letters

a	specific surface area [m^2/m^3]
b	decay rate
k	coefficient
m	mass [kg or g]
n	number of fish
r	reaction rate (intensive/volumetric) [$g/m^3\,d$]
r_o	respiration rate [$g/kg\,d$]
t	time [h or d]
w	fish body weight [kg]

Capital letters

A	area [m^2]
C	concentration [g/m^3]
J	flux [$g/m^2\,d$], cost function
K	Monod constant [g/m^3], diffusion coefficient [m/d or $1/m\,d$]
L	biofilm thickness [mm]
Q	volume flow rate [m^3/d]
R	reaction rate (extensive/total) [g/d]
S	concentration of soluble species [g/m^3]
T	temperature [°C]
Y	yield
V	volume of a tank [m^3]
V_b	volume of bulk liquid in a tank [m^3]
V_w	volume not occupied by fish or carriers [m^3]
X	concentration of particulate species [g/m^3]

Greek letters

α	tuning parameter
β	tuning parameter
ϵ	porosity
μ	maximum growth rate
ν	stoichiometric coefficient, correction factor
ρ	density [kg/m3], process rate [$g_{COD}/m^3\,d$]
τ	time constant, residence time [h]

Subscripts

a	attachment, ammonification
b	bulk
c	biofilm attached to carrier
d	detachment
g	gas
h	hydrolysis
i	component i
p	particulate
H	heterotrophs
A	autotrophs
AOB	ammonia oxidizing bacteria
NOB	nitrite oxidizing bacteria

Superscripts

S	for some soluble species
X	for some particulate species
$*$	saturation

Contents

CHAPTER 1

Introduction

As the world's fisheries are becoming depleted, aquaculture – the farming of fish and aquatic crops such as kelp and algae – is becoming increasingly attractive. Aquaculture is traditionally carried out in natural bodies of water, but an alternative is land-based farming in tanks or raceways, which has particularly high potential when coupled with water treatment to form a recirculating aquaculture system (RAS) where the water is reused to a high degree. Recirculating aquaculture can also be practiced in water-borne closed or semi-closed cages. There are also land-based flow-through systems, which differ from a RAS in that water is not treated to any significant degree and therefore lack many of the sustainability advantages. The different options for aquaculture all carry benefits and drawbacks in terms of cost, environmental impact and requirements of locality. Recirculating systems have the additional difficulty of design and operation of a (possibly very complex) water treatment plant.

This thesis is concerned with computer-based modelling and optimization of recirculating aquaculture systems. The subject was approached from a control engineering and wastewater treatment standpoint, but the text was foremost written with an aquaculture audience in mind.

1.1 Land-based recirculating aquaculture

Recirculating aquaculture in land-based systems has many advantages over traditional open aquaculture and land based flow-through systems. The ability to control the water quality is one obvious feature, where "quality" can mean temperature, oxygen saturation,

carbon dioxide concentration and pH, to name a few important parameters. A typical layout of a RAS is shown conceptually in Figure 1.1. Different techniques to reduce pathogen load can also be incorporated, such as treatment with ozone or ultraviolet radiation.

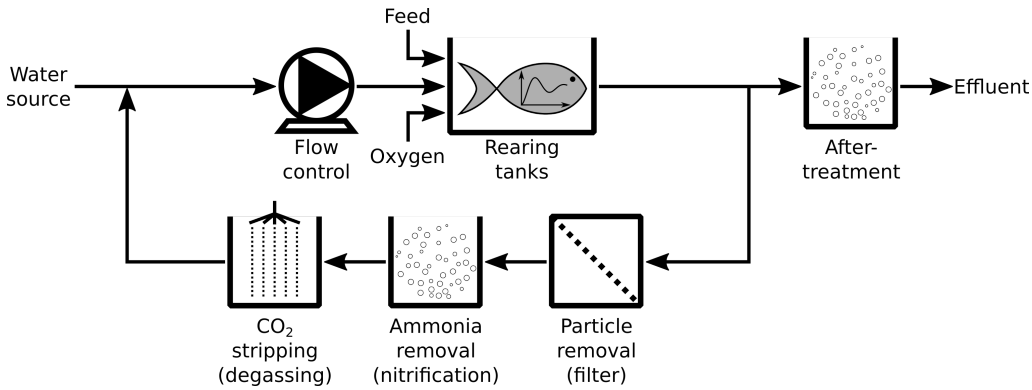


Figure 1.1: A conceptual RAS schematic displaying important components.

Escapes are a significant ecological problem in open cage salmon farming [1], but is for obvious reasons not a serious issue in land based systems. Salmon lice is another problem that troubles traditional salmon aquaculture methods seriously, both economically and environmentally [2], which the isolated nature of a land-based RAS can limit (if not eliminate) the impact of.

The nitrogen-rich emissions to water that are inevitable in cage aquaculture as well as in flow-through land based systems can become a source of eutrophication of the local environment. The considerably lower flow of effluent water that can be obtained in a recirculating system makes after-treatment, such as denitrification reactors for nitrate removal, easier. Constructed wetlands [3] is another choice of after-treatment methodology that has been applied to recirculating systems. Sindilariu *et al.* [4] estimated the land use requirement for wetland after-treatment from intensive trout farming; as an example, they quote a small *flow-through* rainbow trout farm producing 100 t/yr to require about 1330 m^2 of wetland to successfully treat its effluent.

Alternatively, there is also a possibility to include denitrification or other forms of nitrogen removal in the water treatment loop itself, which allows the water exchange rate to be reduced to minute levels. Together, these listed benefits make RAS a promising technology in providing fish for a growing population in a sustainable fashion.

1.1.1 Modelling and simulation of recirculating aquaculture systems

Recirculating aquaculture plants are traditionally dimensioned using steady state material balances [5], [6]. However, the nonlinear dynamics of these systems cause components

and conditions to interact in ways not captured in these methods. Because they contain constantly growing animals, they are also always operating under transient conditions. Moreover, the dynamics in these systems, being biological in nature, are incredibly slow. This makes systematic experimental development enormously time consuming even in downscaled plants.

Simulation of *nonlinear* and *dynamic* aquaculture models could potentially be used both to plan new systems and for improving the operation of existing plants. Mathematical optimization could also be exploited to automatically and optimally size a RAS based on user specifications on e.g. production volume and water treatment topology. Dynamical modelling and simulation is the principal topic of this thesis, and the development of the simulation program LibRAS has been an integral part of the underlying work.

1.2 Thesis outline

The main body of this thesis is divided into three parts. It begins with an introduction to how water treatment in recirculating aquaculture systems typically is approached in Chapter 2. Here, water quality and unit operations are briefly discussed, aiming to familiarize the reader with concepts that are the focus of later chapters. Chapter 3 is concerned with mathematical modelling of recirculating aquaculture systems, beginning with motivations for why computer models are desirable and then moving on to the methods and equations that were used to construct LibRAS. Then, in Chapter 4, the simulator is used to study the performance of different water treatment topologies when applied to different model fish farms.

Chapter 5 ("Future work") discusses some suggested todos that would make LibRAS better, and suggests future research topic. Finally, as an Appendix, a short user guide to the program is given.

CHAPTER 2

Water treatment in recirculating aquaculture

To be able to obtain any meaningful degree of recirculation in a RAS, there must be treatment processes which remove contaminants at nearly the same rate as they enter the system. For the concentration of waste in the system to stay constant, the following equation – a conceptual mass balance – must hold:

$$\text{Production} = \text{Exchange} + \text{Treatment}. \tag{2.1}$$

Intuitively, the better the treatment, the less water needs to be replaced. The left-hand side of the equation is mainly decided by the "fish" aspect of the plant, while the right-hand side is in the domain of the water treatment. Calculating detailed requirements of a particular planned system is a complex task, and is the topic of this thesis.

In this chapter, we discuss the water quality requirements of fish using salmon as an example, then describe the processes used in recirculating aquaculture to treat the water in order to comply with these requirements.

2.1 Water quality requirements

The most important chemical species that must be controlled to maintain fish welfare are dissolved oxygen, carbon dioxide, unionized ammonia (NH_3) and nitrite ($NO_2{}^-$) [7]. Nitrate ($NO_3{}^-$), dissolved organics and particulate matter are also important, but less critically so. Ammonium ($NH_4{}^+$) is a concern due to its equilibrium with ammonia.

Oxygen and carbon dioxide are involved in respiration, while ammonia is also excreted by the fish as metabolic waste. Nitrite and nitrate mainly occur as products from the

treatment processes. Organic waste may originate from undigested feed, fish excrement, or bacterial sludge.

The levels that can be tolerated in the rearing system are dependent on many factors. Different fish species have different innate sensitivities to chemical contaminants and different oxygen requirements, but the water conditions also interact to amplify or diminish the tolerances. For instance, nitrite generally becomes less toxic with increased salinity, and the equilibrium between ammonia and ammonium is dependent on both temperature and pH.

Thorarensen and Farrell [7] states that for post-smolt atlantic salmon (*Salmo salar*) the oxygen saturation should be kept above 80 % (but closer to 100 % is preferred), CO_2 should be below $10\,\mathrm{g/m^3}$, nitrite below $0.1\,\mathrm{gN/m^3}$ and ammonia below $0.012\,\mathrm{gN/m^3}$.

2.2 Physical water treatment

Physical water treatment are those methods in which chemical species are conserved (no reactions take place), such as filtering. They are used to remove particles and to control dissolved gas levels.

2.2.1 Gas transport

Oxygen, nitrogen and carbon dioxide are all important species in fish farming. The high stocking density of fish typically seen in aquaculture results in a high volumetric consumption of oxygen, which in the case of land-based systems must be provided through technical means. A large production of carbon dioxide follows from the fish respiration, which without removal can accumulate to concentrations lethal to the fish [8]. Removal of CO_2 and addition of oxygen are therefore critically important operations in intensive aquaculture.

Degassing of CO2

The carbon dioxide respired dissolves into the water and engages in a complex equilibrium:

$$\mathrm{CO_2(aq) + H_2O \rightleftharpoons H_2CO_3 \rightleftharpoons HCO_3^- + H^+ \rightleftharpoons CO_3^{2-} + 2\,H^+} \tag{2.2}$$

The equilibrium concentrations are a function of the pH value, as is shown in Figure 2.1 [9]. In oceans and in the pH range normally occurring in aquaculture, the relative abundance is shifted strongly towards HCO_3^-, but as more carbon dioxide is added, the pH drops and the CO_2 level rises. With intensive farming the CO_2 concentration can approach dangerous levels [7], and it is possible that specific equipment is required to remove excess gas. Degassing of CO_2 is done by providing ample contact area between water and fresh air in some device. Either air bubbles can be passed through water,

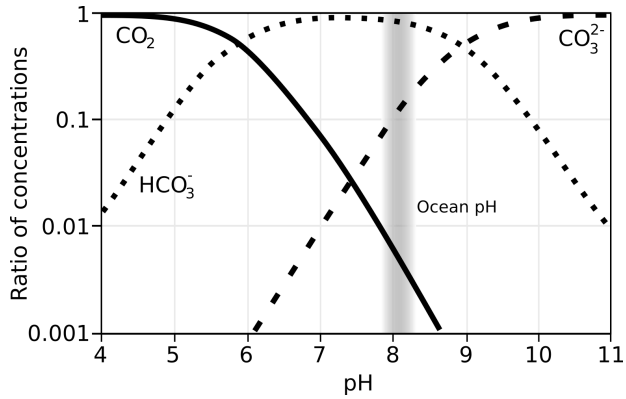


Figure 2.1: Relative concentration of carbonate species as a function of pH [9]. The carbonate equilibrium is dependent on pH, but in a range close to neutral the bicarbonate anion dominates. The shaded area represents ocean pH (≈ 8.1).

or water can be trickled through moving air. Both methods require an expenditure of energy, either as compression work to create bubbles or as pump work to lift the water and, optionally, fan work to move the air.

Aeration and oxygenation

At 15 °C, the saturation concentration for oxygen gas in pure water is $10\,\mathrm{g/m^3}$. Salmon should according to Thorarensen and Farrell [7] be kept at $8\,\mathrm{g/m^3}$ or higher. The small concentration difference means that the driving force for gas transfer is small, and a large interface area between gas and liquid is needed. For other species that are kept at lower levels of dissolved oxygen, the driving force may be larger which simplifies the technical problem of adding enough oxygen to the water stream.

The source of the oxygen can be compressed air, O_2-enriched compressed gas produced on site, or pure O_2 delivered either as compressed gas in cylinders or as a cryogenic liquid. The richer the source is in oxygen, the more efficient the gas transfer becomes, but all oxygenation methods have their downsides. If compressed air is used, care must be taken to avoid too high nitrogen supersaturation as it leads to gas bubble disease which kills fish [10]. With pure oxygen, the main concern is instead to use efficient equipment as not to waste the precious gas. Examples of oxygenation devices are U-tube oxygenators, Speece cones, and low-head oxygenators. Being a powerful oxidizer, pure oxygen also becomes a fire hazard.

2.2.2 Particulate removal

Mechanical treatment, e.g. sieving, filtration or settling, is used to remove particulate materials from the waste stream. In the context of fish farms, the particulates primarily

consist of excrement and undigested feed. Usually, a fairly large part of the particulates are collected at the bottom of the fish tanks. The remaining particles, or at least those above a certain size, are then removed by filtration. Drum filters are a popular choice of equipment, though it is difficult to tell if this has been shown to be the best practice or simply is due to tradition. Band, sand or disc filters are other options.

2.3 Biological water treatment

Dissolved substances like ammonia are, in traditional municipal water treatment as well as in most RAS, handled through biological water treatment, where microbes are employed in technical systems to convert dangerous or unwanted species into less problematic forms. The microbes are usually biofilm-forming bacteria, and for water treatment purposes they are generally categorized as heterotrophic (those that feed on external organic carbon) or autotrophic (those that build their biomass from inorganic carbon). In an environment suitable for heterotrophs, i.e. where readily biodegradable carbon is available, they will typically out-compete the autotropic species and dominate in the community due to their more energetically favourable nutrition strategy [11]. Autotrophic communities are often desirable and creating a favourable environment for them is then of great importance to the designer and operator of the treatment plant.

For water treatment purposes, heterotrophs are employed to remove organic carbon and nitrate, and autotrophs used to convert ammonia into less toxic nitrogen species.

2.3.1 Organic waste

All the energetic components of a fish feed (carbohydrates, fat and proteins) contain a significant fraction of carbon. When fish are fed, the carbon added to the fish tank either ends up in fish biomass, as carbon dioxide (by respiration), as undigested feed lost in the water or as excreted substances after digestion.

Because the organic carbon in the latter two phases is present in many different molecules, its concentration is often measured and expressed as chemical oxygen demand, COD, or biological oxygen demand, BOD. These are measures of how much oxygen is required to fully oxidize all the organic carbon present using either a standard chemical reagent (COD) or microbial degradation (BOD) [12]. Determining COD in a sample typically requires the use of hazardous chemicals such as Cr(VI) compounds, but is a relatively fast method compared to BOD measurements which take several days. Instrumental analysis also allows the measurement of Total Organic Carbon (TOC) which is another measure for the content of organic carbon in a sample. In contrast to "oxygen demand" methods, TOC is based on a measurement of how much carbon dioxide is formed when a sample is fully oxidized. As the modelling work is founded on Activated Sludge Model no. 1 [13], where organic carbon is expressed as COD, this is the measure used in the remainder of the thesis.

Because organic material interferes with the ammonia removal, it is usually in the interest of the operator to keep COD levels low even if fish generally are quite tolerant to dissolved organics. Fine suspended solids should, however, not be allowed to accumulate in the system as they may be detrimental to fish health [7].

2.3.2 Nitrogenous waste

Ammonia, ammonium, nitrite and nitrate are all important nitrogenous species in aquaculture. Ammonia and nitrite exhibit significant toxicity to fish, while ammonium and nitrate are less problematic. Controlling the equilibrium between ammonium and ammonia is therefore very important in an aquaculture setting. The sum of ammonium and ammonia is called Total Ammonia Nitrogen, TAN, and removal of these compounds is one of the key processes in treatment both of municipal waste and in RAS. Nitrification is the most common process employed for this purpose.

Ammonia removal – Nitrification

In an environment scarce in organic carbon, autotrophic *nitrifiers* can oxidize nitrogen compounds like ammonia to produce energy for their growth. The multi-step process called nitrification converts ammonium, via intermediates including nitrite, into nitrate:

$$2\,NH_4^+ + 3\,O_2 \longrightarrow 2\,NO_2^- + 2\,H_2O + 4\,H^+ \tag{2.3}$$

The first step – nitritation – is performed by "ammonia oxidizing bacteria", AOB. They are typically considered to be of the genus *Nitrosomonas* [11]. As the reaction above indicates, this is an acidifying process which will consume alkalinity in the system.

Next, the formed nitrite is further oxidized by NOB, "nitrite oxidizing bacteria" like *Nitrobacter* and *Nitrospira*, into nitrate:

$$2\,NO_2^- + O_2 \longrightarrow 2\,NO_3^- \tag{2.4}$$

Because nitrite is very toxic to fish, it must not be allowed to accumulate and it is therefore critical that both steps of the nitrification functions well.

Nitrate removal – Denitrification

The production of nitrate in the nitrification will cause this compound to accumulate in a closed system unless the nitrate is treated as well. Depending on the amount of water that is exchanged, the concentration of nitrate may eventually become problematic. Davidson *et al.* [14] tested different nitrate levels on rainbow trout (*Oncorhynchus mykiss*) and found adverse effects at chronic levels above 80–100 gN/m^3. In another study [15], atlantic salmon was not found to display any detrimental effects on growth performance or health at these levels. Regardless of its effect on fish health, nitrate discharge is problematic from an environmental perspective and regulations may put a limit on the

effluent nitrate concentration. Nitrate accumulation can be combated by introducing denitrification, a process carried out by (facultative) anaerobic heterotrophs [16]. In an environment low in oxygen but rich in carbon, i.e. the opposite of that required for nitrification, certain bacteria – denitrifiers – may use nitrate for their respiration instead of oxygen. This reduces the nitrate in a series of steps ending in dinitrogen, N_2.

$$NO_3{}^- \longrightarrow NO_2{}^- \longrightarrow NO \longrightarrow N_2O \longrightarrow N_2 \tag{2.5}$$

Nitrification and denitrification thus have opposite requirements – nitrification demands plenty of oxygen and low levels of organic carbon, while for denitrification an anaerobic environment with readily biodegradable carbon is necessary. The anaerobic environment is typically obtained by having heterotrophs consume most of the oxygen. If one locates the nitrification train prior to the anoxic section, there is no carbon available for this to happen, and it must then be added from an external source (typically in the form of acetate or methanol).

If the denitrification is not complete, owing for instance to poor control of the oxygen concentration, nitrous oxide (N_2O) may instead be produced [17], [18]. It is a potent greenhouse gas, which means that this is something that best should be avoided.

Ammonia assimilation

Heterotrophic bacteria also use nitrogen in aerobic environments, not as an energy source but in their biomass to build proteins. Growth of heterotrophic biomass therefore also removes TAN from the water, but at the cost of both oxygen and carbon. The production of bacterial sludge is also generally undesired, so unnecessary "feeding" of heterotrophs is usually avoided if possible.

Anammox

Anammox, *anaerobic ammonia oxidation*, is another TAN removal process which has the advantage that it proceeds without oxygen in the following manner:

$$NH_4{}^+ + NO_2{}^- \longrightarrow N_2 + 2\,H_2O \tag{2.6}$$

The anaerobic process is beneficial because aeration of nitrification reactors requires significant compression work. With anammox, only a fraction of the oxygen is needed to provide the nitrite (by AOB) as per Reaction 2.3. As the product of the reaction is molecular nitrogen, the issue of nitrate accumulation is also remedied, and without nitrate production there is no need for carbon to drive denitrification. These benefits make anammox desirable, and although there are promising demonstrations [19] the technology is not yet mature enough for reliable employment in cold aquaculture streams with relatively low TAN levels compared to most municipal wastewater.

2.3.3 Bioreactors

The technical equipment used to facilitate a biological treatment process is called a bioreactor. Most bioreactors can be divided into two main types: biofilters and activated sludge reactors. In the activated sludge process, bacteria are suspended in free flocs while in biofilters they form a film fixed to some substrate. Because biofilm-based reactors are much more common in aquaculture, we do not futher consider activated sludge in this thesis.

Biofilter designs vary, but they are all based on the principle of providing a large surface area on which biofilm can grow, and (if aerobic) adequate contact between water and air. They can be divided into fixed bed and moving bed types. In a fixed bed biofilter, the growth medium is static. The trickling filter, conceptually drawn in Figure 2.2, is an example of a fixed bed biofilter. Various *submerged biofilter* designs (Figure 2.3) are also common, such as packed beds where the growth medium can be sand, plastic granules, wood chips or specially designed biocarriers. Figure 2.4 shows a photo of a modern plastic biocarrier. If the packing of the carrier medium is low enough to allow movement, and the water is sufficiently agitated by bubbling or stirring, the carrier medium becomes mobile and a moving or fluidized bed results. The *moving bed biofilm reactor* (MBBR), originally introduced by Ødegaard *et al.* [20], is a particular biofilter type using plastic carriers that is advantageous in that it can be well mixed even in an anoxic configuration, which additionally simplifies modelling.

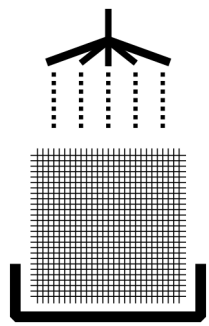


Figure 2.2: The "trickling filter" is an example of a common fixed bed biofilter. Water is sprayed over a rigid structure covered in biofilm and trickles down, by gravity, as a thin layer over the biofilm surface.

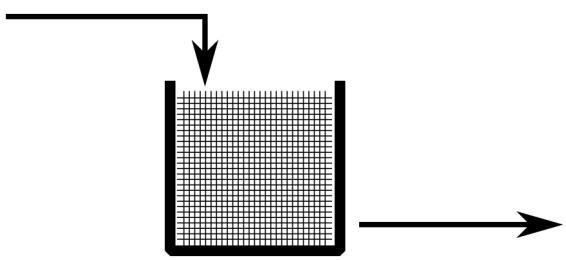


Figure 2.3: Fixed bed biofilters can be constructed with submerged carrier material, either as a rigid construction or a packed bed of individual carrier elements.

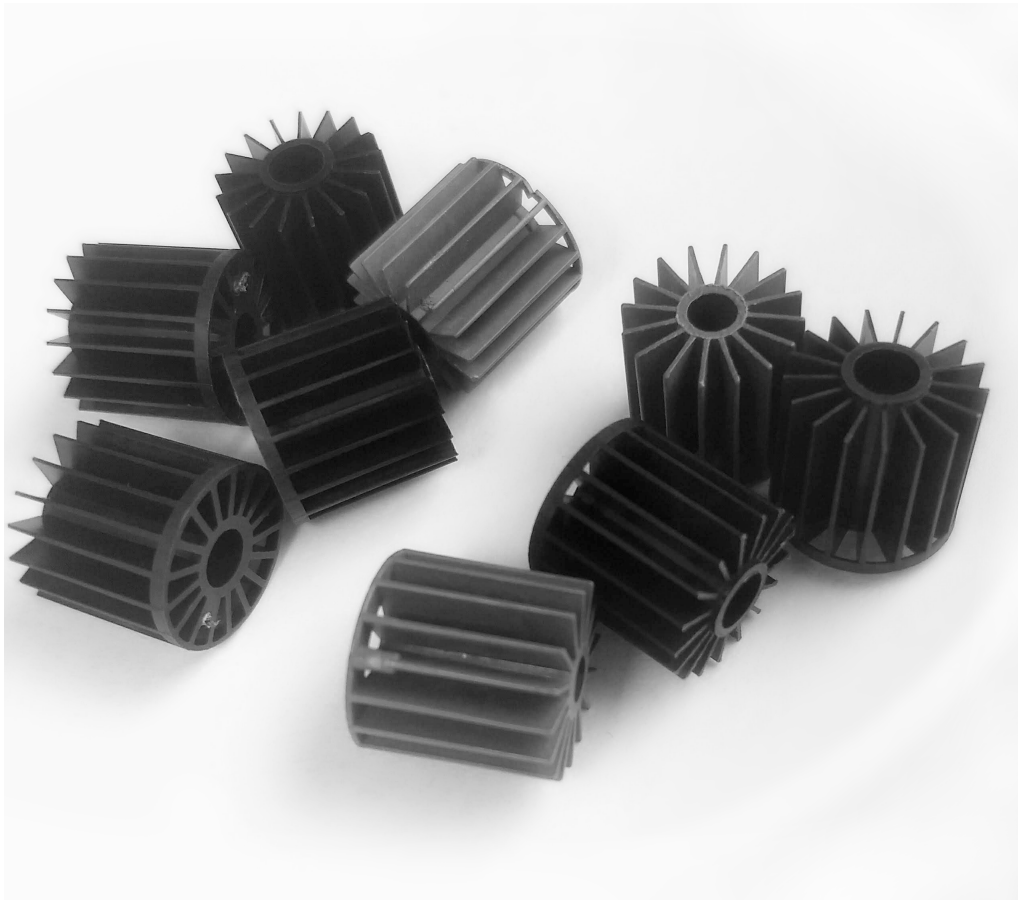


Figure 2.4: Plastic biocarriers. This particular model has a reported surface area of $750\,\mathrm{m}^2/\mathrm{m}^3$.

CHAPTER 3

Recirculating aquaculture system modelling

In aquaculture, both traditional and recirculating, it is highly useful to be able to estimate fish growth. The calculated increase in biomass can be used to decide how much one should feed the fish, if the feed conversion ratio (FCR) is known. *Specific growth rate* (SGR) and *Thermal growth coefficient* (TGC) are two modelling approaches; the latter was used in this work.

Designing a recirculating aquaculture plant also requires modelling of biofilter efficiency and removal rates, in order to give an estimate on the types and sizes of equipment needed. Quite early, Losordo and Westers [21] modelled water treatment in recirculating *aquaculture* specifically (modelling in municipal wastewater treatment began much earlier). Later, continuing on this work, Losordo and Hobbs [5] created a spreadsheet-driven program for sizing the water treatment based on expected nitrogen load. Other computer models have followed; Pedersen *et al.* [22] used the modelling tool AQUASIM [23] to build a prediction model, similarly focusing mainly on TAN and its removal and tuned it to measurements taken from replicated experimental systems. These two computer models were, however, operating under a steady state assumption – a common, but limiting, simplification. FishSim by Wik *et al.* [24] is a *dynamic* recirculating aquaculture simulator built in MATLAB and Simulink (The MathWorks, Inc., Natick, Massachusetts, United States). It is founded on the widespread municipal wastewater treatment model suite ASM [13] and integrates fish growth, digestion/evacuation and water treatment. It is based on this work that the simulation package presented in this thesis – LibRAS – is built.

3.1 Motivations

Wik *et al.* [24] argued for the necessity of integrated dynamic simulations of both fish and water treatment, stating reasons including the tediousness and expense of experimenting on live RAS and the failure of existing models to account for interacting dynamics. The following section aims to repeat and expand on these motivations.

Complementing experiments

Recirculating aquaculture systems, being biological in nature, evolve very slowly. The bacterial colonies in the water treatment adapt to changes over weeks or months; fish growth cycles may range from many months to years. This slowness alone makes it difficult to develop certain aspects of RAS technology experimentally. Down-scaled systems can be set up to do experiments on e.g. a bioreactor, but they fail to account for the high complexity and transient nature of the integrated RAS.

With a computer model that replicates a RAS with sufficient fidelity, "experiments" are ideally as simple as modifying parameters and pushing a button. Results can easily be read out and plotted, and variables that are difficult to measure can be investigated at will. Most importantly, even if the results are inaccurate, simulations are fast, and qualitative knowledge ("if I change this parameter, what happens to the concentration of nitrite in the second anoxic biofilter?") can easily be obtained. A simulator can also be used for operator training or other education, as is customary in many other industries.

To conclude, **simulation of recirculating aquaculture systems, made possible by computer models, is a useful tool to gain new and deeper knowledge about the workings of such systems.**

Model complexity

The program by Losordo and Hobbs [5] required the user to specify the TAN removal rate of their nitrification biofilter. As a first approximation, this stationary mass-balance approach is sound. However, the components in a RAS are complex, interacting in ways that are sometimes not obvious. By including kinetics in the model, some of this complexity is captured at the cost of a larger, more complex system of equations that is more difficult to solve.

In essence, **the dynamical interactions between fish, feeding and microbiology affects the treatment system performance, but is not accounted for in static models using fixed waste removal rates.**

Optimal design

Apart from analysis, another common use-case for models is plant design. With the computing power available today even on a modest desktop computer, running optimization programs on a full-scale RAS model is fully feasible. This allows us to specify a goal in

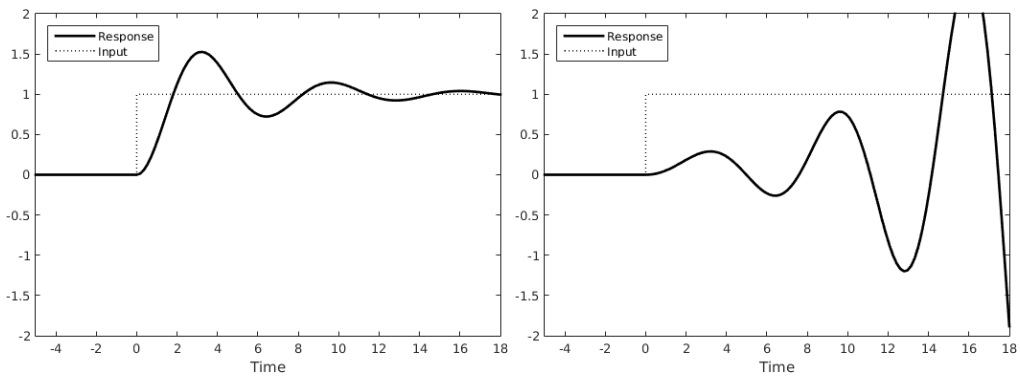
the form of a mathematical function and let the computer search for the solution that minimizes or maximizes this function, essentially automating the design of the system. A natural choice of goal (or cost) function is economic, so that the algorithm for instance minimizes the sum of (weighted) investment and running costs per produced mass of fish. Such a cost function typically requires considerable effort to construct, however, so other formulations not directly reflecting economy can also be attractive.

The cost function together with *constraints* specify the desires of the designer, which are then passed to an optimization solver which attempts to find the best design, taking into account all the interactions described in the model.

With good integrated models for fish culture and water treatment, design (sizing) of the water treatment plant can potentially be done automatically through mathematical optimization.

Feedback and stability

In the field of automatic control, the *stability* of a system is a core concept. A stable system will converge to a steady value if it is left to evolve, while an unstable system will diverge from its current operating point, its states possibly going towards infinity. Figure 3.1 illustrates this difference. In an aquaculture system, instability would manifest as biofilter collapse, uncontrollable concentration fluctuations and so forth. Another key

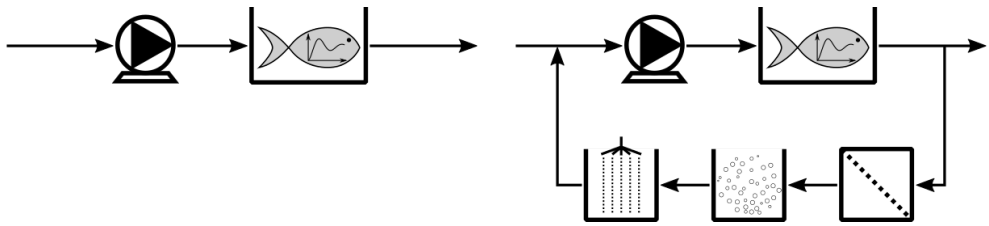


(a) Stable system **(b)** Unstable system

Figure 3.1: Step responses of two example systems (second order) beginning at time $t = 0$. Stable dynamics (left) converge to the change in input (dotted line), while unstable dynamics (right) cause a divergent behavior with oscillations that grow uncontrollably in amplitude.

concept is *feedback*; it can be exemplified as the difference between a once-through system and a recirculating one (as illustrated in Figure 3.2). If we consider the water intake to be the input to the system, the conditions in the fish tank of a flow-through plant are determined by the parameters of this water and the fish. On the other hand, in a

recirculating aquaculture system the current conditions are also influenced by the *past output* via the recirculation loop.



(a) System without feedback **(b)** System with feedback

Figure 3.2: An illustration of feedback – in a recirculating aquaculture system, the current conditions are influenced by the past through the recirculation loop as well as by the input (the make-up water). In a flow-through system, only the input matters.

Feedback, in the form of a control system, has the possibility both to stabilize an unstable plant (a key application of control theory), and destabilize a stable one. The latter typically happens when the control engineer desires his controllers to work faster than the physical system can react. A series of oscillations growing in amplitude results, and at some point the system must be shut down, is destroyed, or proceeds in other undesired directions.

It has not been formally proven whether a recirculating aquaculture system is stable or not, and we may never see such a proof. Nevertheless, stability is an important concept because we want our water treatment plants to behave predictably. In automatic control, stability is usually investigated for a mathematical model of the real system. Even if the physical system is apparently stable, through mathematical proof or observation, introduction of feedback loops such as pH control or addition of organic compounds to power denitrification may alter this.

For these reasons, **control engineering considerations such as stability motivate the construction of thorough, integrated models for recirculating aquaculture.**

3.2 LibRAS

The simulation package LibRAS (`https://github.com/FishSim/LibRAS`) for recirculating aquaculture is written as a Modelica library and developed in the free simulation environment OpenModelica [25]. It is the successor to FishSim and implements many of the same equations, but does so in a new modelling suite which was found to give far better performance and "robustness", i.e. the ability to simulate different variations of the RAS concept without issue. Further improvements over FishSim is the inclusion of denitrification, the separation of NO_x^- into NO_2^- and NO_3^- and autotrophic bacteria

into AOB and NOB, automatic interpolation of biofilm parameters, and simultaneous simulation of fish and waste treatment models.

Both FishSim and LibRAS use dynamic material balances to calculate the production of waste components and their respective concentrations throughout the system. A growth model based on thermal growth coefficient (TGC) is used together with a dynamic feeding and evacuation model, which transfers feed input to a delayed excretion response, where the delay and dynamics depend on fish size.

The water treatment models are derived from the widespread ASM1 model [13] with supplements suggested by Wik *et al.* [24] and extended with denitrification [26]. The simulator uses continuously stirred biofilm reactor (CSBR) models for its bioreactor components, which is a structure that can approximate many common biofilter designs [27].

Additionally, LibRAS is built with Modelica's Fluids library, which provides mass and energy balances for the hydraulics and thermal dynamics. As a consequence, the simulator is almost fully equipped to model energy flows in recirculating aquaculture plants including heating/cooling, pump work, pressure drop in pipes, et cetera. Compression work for aeration is however still not implemented.

3.3 Models in LibRAS

The modelling of a RAS can roughly be broken down into three parts: the fish (growth, feeding and waste excretion), the fluid (movement and energy transfer in and between tanks) and the bioreactions. The next section aims to explain the way these are modelled in LibRAS.

3.3.1 Fish growth

Fish are assumed to grow according to the Thermal Growth Coefficient (TGC) model. This model makes the following approximations:

- Fish body weight is proportional to body length cubed.
- The growth rate is only affected by the instantaneous temperature, and the relationship is linear with proportionality constant TGC.

If w_2 and w_1 denotes body weight in grams at two different times, T the temperature in °C at which the fish has been kept, and t is the time difference in days, then the TGC is calculated as

$$TGC = 1000 \frac{w_2^{1/3} - w_1^{1/3}}{T \cdot t}. \tag{3.1}$$

The TGC is typically reported without a unit, but in the formulation above it would be of dimensions $\mathrm{g}^{\frac{1}{3}}/\mathrm{d} \cdot {}^\circ\mathrm{C}$ with the cubic root of mass again being proportional to body

length. The equation can be solved for w_2 to find the expected body weight (in g) after time t

$$w_2(t) = (w_1^{1/3} + TGC \cdot T \cdot t/1000)^3, \tag{3.2}$$

or differentiated with respect to t to find the instantaneous growth rate in g/d, i.e.

$$\dot{w}(t) = \frac{3TGC \cdot T}{1000}(w_1^{1/3} + TGC \cdot T \cdot t/1000)^2. \tag{3.3}$$

Next, we name the number of fish in a tank at a specific time $n(t)$. Assuming that all fish grow identically, the mass of fish in the tank is then $m(t) = w(t)n(t)$ where $w(t)$ is the current body weight according to Equation 3.2. By differentiating this, we arrive at an expression for the accumulation of fish biomass:

$$\frac{\mathrm{d}}{\mathrm{d}t}m(t) = n(t)\dot{w}(t) + w(t)\dot{n}(t) \tag{3.4}$$

As this expression models the rate of change in fish mass, we can link it (through the feed conversion ratio) to the amount of feed that is consumed. The information obtained about feed and fish mass is then used to calculate the rate of waste excretion.

The number of fish $n(t)$ can also be modelled dynamically. The simplest dynamical model is to assume that the number of fish is not an integer but real number, in which case a rate of death (e.g. 2 % per production cycle) can be translated into an exponential decay on the form

$$n(t) = n_0 \mathrm{e}^{-kt} \tag{3.5}$$

where n_0 is the number of fish at the beginning of the production cycle t_p and k is a rate constant, determined from the length of the production cycle and the percentage p of deaths:

$$k = -\frac{\ln(1 - p/100)}{t_\mathrm{p}}. \tag{3.6}$$

At the time of writing, LibRAS supports two different rearing modes:

- A ”smooth” mode where grading is assumed to take place at very short intervals, so that the production of grown fish is almost a continuous process. Feed is also added continuously throughout the day at a constant rate. The resulting waste production is then constant in time, which gives very fast calculations. Note that the water treatment model (biofilm growth, accumulation of waste, et cetera) is still dynamical in this mode.

- A non-smooth mode, where complete gradings are performed with arbitrary intervals and where temporal feeding regimes can be chosen by the user. This leads to a fluctuating mass of fish in the system and a transient waste production. While a more accurate representation, it leads to slower simulations.

After a long time, the biofilm stabilizes around a quasi-steady state even in the transient rearing mode, with periodic flucuations that correspond to the variation in fish biomass. Figure 3.3 shows the concentration profile between two gradings while in this quasi-steady state.

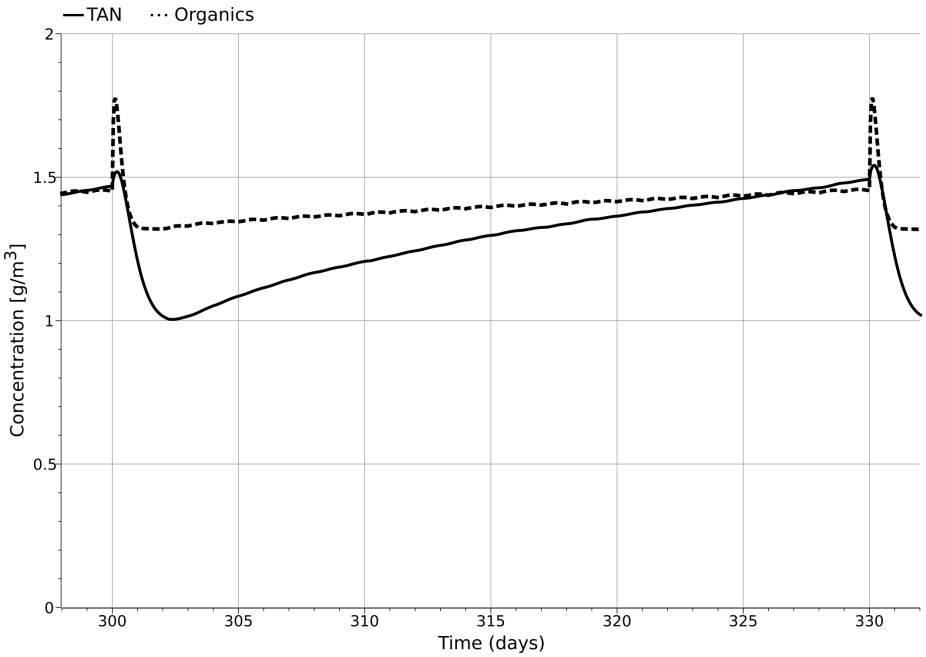


Figure 3.3: Typical transient behavior between two gradings. The spikes at 300 and 330 days are the result of overfeeding that occur when the largest fish are suddenly removed. The TAN quickly drops as the feeding is adjusted, but it takes a few days for nitrification to bring the concentration down to a minimum.

3.3.2 Feeding and evacuation

For the development of FishSim, Wik *et al.* [24] formulated a dynamic model of the waste excretion from fish, based on elementary knowledge about linear dynamical systems and time series measurements of fish excretion response after feeding. It was assumed that the production of waste could be described by second order dynamics and that intense feeding took place during a short time. The waste excretion could then be approximated as an impulse response of the type shown in Figure 3.4.

For a waste component i, for instance TAN, an impulse response with this shape can

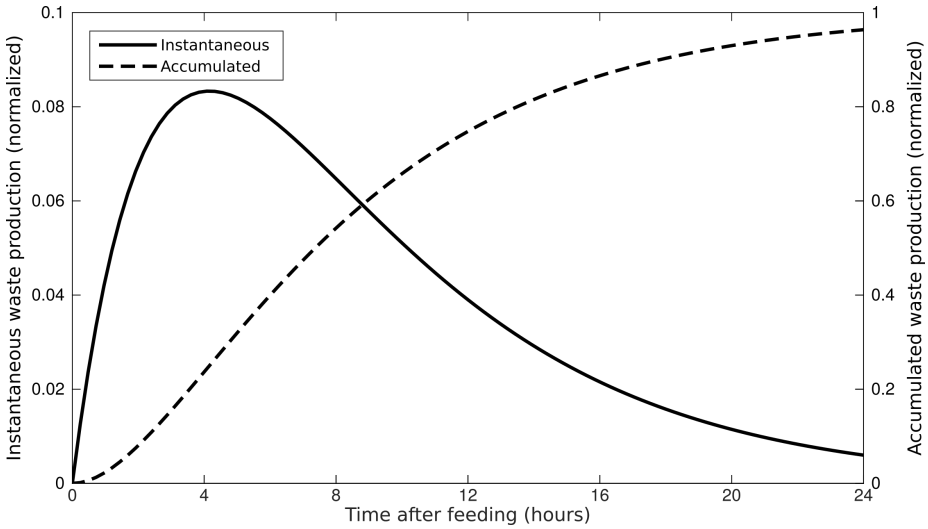


Figure 3.4: Production of waste from a fish after impulse (very short and intense) feeding. The dynamics are of second order with time constants $\tau_1 = 1\,\mathrm{h}$, $\tau_2 = 2\,\mathrm{h}$. The curves have been normalized to a total accumulated waste production of 1 unit.

be obtained from the following linear dynamical model:

$$\tau_1 \frac{\mathrm{d}}{\mathrm{d}t} x_i(t) = -x_i(t) + k_i F(t) \tag{3.7}$$

$$\tau_2 \frac{\mathrm{d}}{\mathrm{d}t} y_i(t) = -y_i(t) + x_i(t) \tag{3.8}$$

$$\tilde{F}_i(t) = y_i(t) \tag{3.9}$$

The time constants τ_1 and τ_2 determine the shape of the response and can be thought of as the hydraulic retention times of two series-connected mixed tanks that represent the gastrointestinal tract; Figure 3.5 illustrates this idea. We roughly estimate these as depending linearly on fish size. $F(t)$ is a function which describes the intake of feed, $\tilde{F}(t)$ is the output of digested feed, and x and y represent the internal state in the two intestine compartments. Finally, the coefficient k_i allocates the feed to the different waste components, and must be estimated using material balances. The distribution of feed components (carbon, nitrogen and inert material) into the different phases (feed loss, fish tissue, waste and respired gases) and components (readily biodegradable organics, TAN, etc.) is described as a "waste matrix". We use the same distribution as Wik *et al.* [24], which is presented in Table 3.1. What the different components represent is explained in Table 3.2. Once the production of waste is known, the information is sent to the water treatment model.

Table 3.1: Waste is distributed into different fractions according to the waste matrix. I is the inert matter content, COD is carbon content as COD, N is nitrogen content and r_o is respiration rate.

Component kg generated	**Lost feed** per kg lost feed	**Digested feed** per kg digested feed	**Growth** per kg fish/d	**Respiration** per kg fish
Soluble components (S)				
I	$0.5I_{\text{feed}}$	$0.5I_{\text{feed}}$	$-0.5I_{\text{fish}}$	
S	$0.7COD_{\text{feed}}$	$0.15COD_{\text{feed}}$	$-0.15COD_{\text{fish}}$	$-0.15r_o$
O				$-r_o$
NO2				
NO3				
NH		$0.5N_{\text{feed}}$	$-0.5N_{\text{fish}}$	
ND	$0.5N_{\text{feed}}$	$0.2N_{\text{feed}}$	$-0.2N_{\text{fish}}$	
Alk				
CO2				$(44/32)r_o$
Particulate components (X)				
I	$0.5I_{\text{feed}}$	$0.5I_{\text{feed}}$	$-0.5I_{\text{fish}}$	
S	$0.3COD_{\text{feed}}$	$0.15COD_{\text{feed}}$	$-0.15COD_{\text{fish}}$	$-0.15r_o$
BH		$0.5COD_{\text{feed}}$	$-0.5COD_{\text{fish}}$	$-0.5r_o$
AOB				
NOB				
p		$0.2COD_{\text{feed}}$	$-0.2COD_{\text{fish}}$	$-0.2r_o$
ND	$0.5N_{\text{feed}}$	$0.3N_{\text{feed}}$	$-0.3N_{\text{fish}}$	

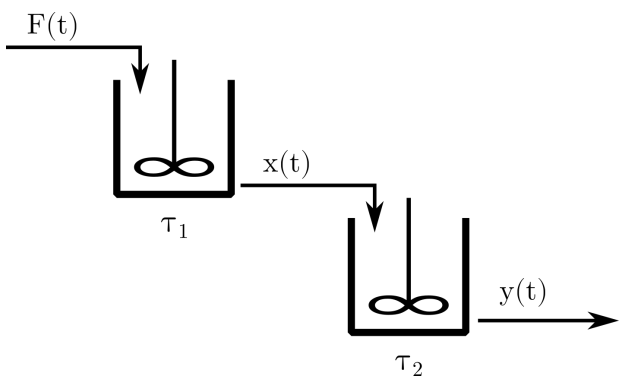


Figure 3.5: The intestine model can be visualized as two mixed tanks in series with hydraulic retention times τ_1 and τ_2. $F(t)$ is the feed input through the mouth, $x(t)$ is an internal state in the intestine and $y(t)$ is the produced waste.

3.3.3 Biological treatment

The basis for the water treatment modelling is Activated Sludge Model no. 1 [13], in which waste components are grouped according to their role in the biological processes. Substances are categorized as either soluble, with concentrations denoted by the variable S_i, or particulate, with concentration variable X_i (for component i). The modelled "species" and their shorthand indices are shown in Table 3.2. A concentration variable denoted C_i can be either for a soluble or a particulate component, in those cases where the same equation is valid for both.

Table 3.2: Waste components

Index	Description	Index	Description
Soluble components (S)		**Particulate components (X)**	
I	inert material	I	generic inert material
S	biodegradable organics	S	biodegradable organics
O	dissolved oxygen	BH	heterotrophic bacteria
NO2	nitrite	AOB	ammonia-oxidizing bacteria
NO3	nitrate	NOB	nitrite-oxidizing bacteria
NH	total ammonia nitrogen	p	inert material from biomass decay
ND	organically bound nitrogen	ND	organically bound nitrogen
Alk	alkalinity		
CO2	dissolved carbon monoxide		

Bacterial abundance is expressed in weight of biomass (as COD). All concentrations except for alkalinity are in mass per unit volume (g/m^3). Alkalinity is instead expressed in mol HCO_3^--equivalents per unit volume.

The Continuous Stirred Biofilm Reactor

The biofilters are modelled as Continuous Stirred Biofilm Reactors (CSBRs), an extension of the classic CSTR chemical reactor model [27]. A CSBR model has several ideally mixed compartments, one of which represent the bulk liquid. From the bulk, components can diffuse into another compartment representing the topmost layer of the biofilm. Particles (including bacteria) in the bulk can attach and detach from the biofilm. The bulk also interacts with (dispersed) air, allowing exchange of gases. The total volume of all compartments is constant, but the volume distribution may vary as the biofilm layer(s) grow. In this work, we have so far only implemented a single-layered biofilm model.

In the bulk compartment, the material balance for component i has the form

$$\frac{\mathrm{d}(V_\mathrm{b}C_i)}{\mathrm{d}t} = Q(C_{i,\mathrm{in}} - C_i) + R_i - AJ_i + A_\mathrm{g}J_{\mathrm{g},i} \tag{3.10}$$

where C_i is the concentration of component i in the compartment, $C_{i,\mathrm{in}}$ is the concentration in the inflow, V_b is the volume of the bulk compartment, Q is the liquid flow rate, R_i is the production or consumption of the component, A is the area of the biofilm

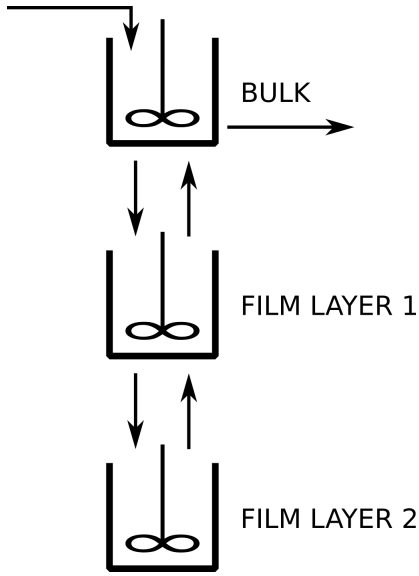


Figure 3.6: The principle behind the CSBR model. All compartments are ideally mixed, and components diffuse between them. The number of biofilm layers can be expanded or reduced. In each compartment, reactions take place homogeneously.

in contact with the liquid, and the flux J_i is the transport rate of component i into the biofilm. Similarly, A_g is the interface area between the liquid and a well-mixed gas with corresponding gas transport rate $J_{\mathrm{g},i}$, which is non-zero only for gaseous species (O_2 and CO_2). The transport between a gas phase and a well-mixed liquid can be modelled by the relationship

$$J_{\mathrm{g},i} = k_{\mathrm{L},i}(C_i^* - C_i), \tag{3.11}$$

where $J_{\mathrm{g},i}$ is the flux into the liquid (e.g. in $\mathrm{g/m^2\,s}$), $k_{\mathrm{L},i}$ is a mass transfer coefficient, and $C_i^* - C_i$ is the difference between saturation and bulk concentration in the liquid. Multiplying with an interface area A_g gives the amount of gas being transferred in unit time, e.g. g/s. It is often difficult to estimate both k_L and A_g accurately, so these parameters are often lumped into the single variable $k_\mathrm{L}A_\mathrm{g}$. It is zero for all non-gaseous species.

If we let L be the thickness of the biofilm, then the product LA is the volume occupied by the biofilm. If V_w is the volume in the tank not occupied by biocarriers, the total volume of the liquid in the bulk phase is $V_\mathrm{b} = V_\mathrm{w} - LA$. Additionally, the interface area for gas-liquid transfer is $V_\mathrm{b} \cdot a = (V_\mathrm{w} - LA)a$, where a is a measure of bubble size and abundance in $\mathrm{m^2/m^3}$. By letting r_i be the production or consumption per unit volume and combining these we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(V_\mathrm{w} - LA)C_i = Q(C_{i,\mathrm{in}} - C_i) - AJ_i + (V_\mathrm{w} - LA)(r_i + aJ_{i,\mathrm{g}}) \tag{3.12}$$

and by substituting the expression for the gas flux $J_{i,\mathrm{g}}$,

$$\frac{\mathrm{d}}{\mathrm{d}t}(V_\mathrm{w} - LA)C_i = Q(C_{i,\mathrm{in}} - C_i) - AJ_i + (V_\mathrm{w} - LA)(r_i + k_{\mathrm{L,i}}a[C_i^* - C_i]). \tag{3.13}$$

Because the biofilm thickness L also is a function of time, the left side expression is expanded using the product rule for derivatives according to

$$\frac{\mathrm{d}}{\mathrm{d}t}(V_\mathrm{w} - LA)C_i = V_\mathrm{w}\frac{\mathrm{d}}{\mathrm{d}t}C_i - A\frac{\mathrm{d}}{\mathrm{d}t}LC_i = V_\mathrm{w}\frac{\mathrm{d}C_i}{\mathrm{d}t} - A\frac{\mathrm{d}L}{\mathrm{d}t}C_i - AL\frac{\mathrm{d}C_i}{\mathrm{d}t}. \tag{3.14}$$

Finally, by rearranging, we arrive at

$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = \frac{QC_{i,\mathrm{in}} + (A\frac{\mathrm{d}L}{\mathrm{d}t} - Q)C_i - AJ_i}{V_\mathrm{w} - LA} + r_i + k_{\mathrm{L,i}}a[C_i^* - C_i] \tag{3.15}$$

which is a state equation for the concentration of component i in the bulk that can be implemented in the computer model and solved.

Transport equations

Transport of components from the bulk to the biofilm is a key feature of the CSBR model. It now becomes necessary to differentiate between concentrations of soluble compounds and particulate matter, because their transport equations are different. Let S denote concentrations of soluble components, and X those of particulate components. Indices b and c are used for "bulk" and "carrier", because we only consider biofilm attached to the carrier material.

For a soluble component, we assume transfer between bulk and biofilm to follow the equation

$$J_i^\mathrm{S} = K_\mathrm{x}(S_{i,\mathrm{b}} - S_{i,\mathrm{c}}) \tag{3.16}$$

with the mass transfer coefficient K_x approximated to a constant. For particulate matter, the equation

$$J_i^\mathrm{X} = K_\mathrm{a}X_{i,\mathrm{b}} - K_\mathrm{d}L^2X_{i,\mathrm{c}} \tag{3.17}$$

was used, which Wik [27] found to give detachment rates corresponding to what is common in models of fixed biofilms. Here K_a and K_d are attachment and detachment rate coefficients, and one common value for each is assumed to be valid for all the particulate species. The coefficient K_d is allowed to vary continuously with the bacterial composition of the biofilm, as the physical properties of nitrifying and heterotrophic biofilms are different, according to the formula

$$K_\mathrm{d} = \frac{K_{\mathrm{d,H}} + K_{\mathrm{d,A}}\mathrm{e}^{-k(x-x_0)}}{1 + \mathrm{e}^{-k(x-x_0)}} \tag{3.18}$$

where x is the ratio of heterotrophic bacteria to total bacteria, i.e.

$$x = \frac{X_{\mathrm{BH,c}}}{X_{\mathrm{BH,c}} + X_{\mathrm{AOB,c}} + X_{\mathrm{NOB,c}}}, \tag{3.19}$$

and k and x_0 are tuning parameters shaping the resulting S-curve. When $x = x_0$, K_d is exactly the mean of $K_{\mathrm{d,H}}$ and $K_{\mathrm{d,A}}$. An example is shown in Figure 3.7.

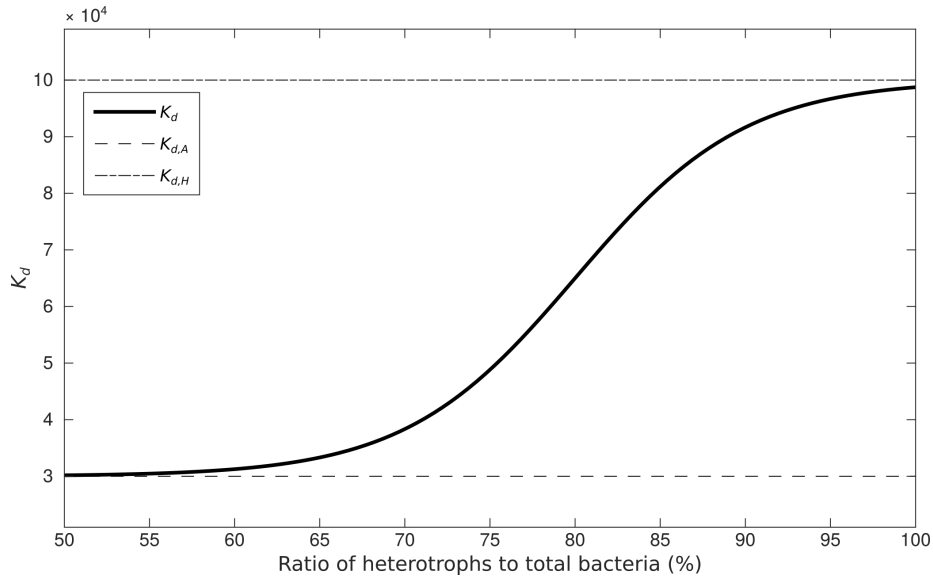


Figure 3.7: An example of the S-shaped interpolation between biofilm parameters. Here, $K_{\mathrm{d,A}} = 30\,000\,\mathrm{m}^{-1}\,\mathrm{d}^{-1}$, $K_{\mathrm{d,H}} = 100\,000\,\mathrm{m}^{-1}\,\mathrm{d}^{-1}$, $x_0 = 0.8$ and $k = 20$.

Biofilm

Because there is no bulk movement of biofilm in the model, the material balances for biofilm components have the following, simpler expressions:

$$\frac{\mathrm{d}}{\mathrm{d}t}(LA\epsilon S_{i,\mathrm{c}}) = AJ_i^{\mathrm{S}} + LAr_i^{\mathrm{S}} \tag{3.20}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(LAX_{i,\mathrm{c}}) = AJ_i^{\mathrm{X}} + LAr_i^{\mathrm{X}} \tag{3.21}$$

We note again that the product LA is the total volume of the biofilm. The parameter ϵ is the porosity of the biofilm, and $LA\epsilon$ is therefore the volume in the biofilm not occupied by particulate material. It is for this "void volume" that we define the concentration of a soluble component, and this causes the small difference between equations 3.20 and 3.21. Similar manipulations to those made on the bulk material balance brings us the

state equations for the concentrations in the biofilm:

$$\frac{\mathrm{d}S_{i,\mathrm{c}}}{\mathrm{d}t} = \frac{1}{L\epsilon}(J_i^{\mathrm{S}} - \epsilon S_{i,\mathrm{c}}\frac{\mathrm{d}L}{\mathrm{d}t}) + r_{i,\mathrm{c}}^{\mathrm{S}} \tag{3.22}$$

$$\frac{\mathrm{d}X_{i,\mathrm{c}}}{\mathrm{d}t} = \frac{1}{L}(J_i^{\mathrm{X}} - X_{i,\mathrm{c}}\frac{\mathrm{d}L}{\mathrm{d}t}) + r_{i,\mathrm{c}}^{\mathrm{X}} \tag{3.23}$$

$$\tag{3.24}$$

Lastly, an expression for how the thickness L of the biofilm varies with time is needed. By letting ρ_X be the density of the particulate matter in the biofilm, it takes the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}LA(1-\epsilon)\rho_X = \sum_i (AJ_i^{\mathrm{X}} + ALr_i^{\mathrm{X}}), \quad i \neq \mathrm{ND} \tag{3.25}$$

The sum is over all particulate components except for X_{ND}, because this quantity is defined in ASM1 to account for nitrogen *in* other substances, and therefore does not occupy any space. Solving for the derivative of L gives

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \frac{1}{(1-\epsilon)\rho_{\mathrm{X}}}\sum_i (J_i^{\mathrm{X}} + Lr_i^{\mathrm{X}}), \quad i \neq \mathrm{ND} \tag{3.26}$$

Reactor dynamics summary

Compiling the equations presented above gives the following dynamics of the biofilm reactor, now lacking only the reaction rates r. They will be presented in the next section.

$$\frac{\mathrm{d}S_{i,\mathrm{b}}}{\mathrm{d}t} = \frac{QS_{i,\mathrm{in}} + (A\frac{\mathrm{d}L}{\mathrm{d}t} - Q)S_{i,\mathrm{b}} - AJ_i^{\mathrm{S}}}{V_{\mathrm{w}} - LA} + r_{i,\mathrm{b}}^{\mathrm{S}} + (k_{\mathrm{L}}a)_i[S_i^* - S_{i,\mathrm{b}}] \tag{3.27}$$

$$\frac{\mathrm{d}X_{i,\mathrm{b}}}{\mathrm{d}t} = \frac{QX_{i,\mathrm{in}} + (A\frac{\mathrm{d}L}{\mathrm{d}t} - Q)X_{i,\mathrm{b}} - AJ_i^{\mathrm{X}}}{V_{\mathrm{w}} - LA} + r_{i,\mathrm{b}}^{\mathrm{X}} \tag{3.28}$$

$$\frac{\mathrm{d}S_{i,\mathrm{c}}}{\mathrm{d}t} = \frac{1}{L\epsilon}(J_i^{\mathrm{S}} - \epsilon S_{i,\mathrm{c}}\frac{\mathrm{d}L}{\mathrm{d}t}) + r_{i,\mathrm{c}}^{\mathrm{S}} \tag{3.29}$$

$$\frac{\mathrm{d}X_{i,\mathrm{c}}}{\mathrm{d}t} = \frac{1}{L}(J_i^{\mathrm{X}} - X_{i,\mathrm{c}}\frac{\mathrm{d}L}{\mathrm{d}t}) + r_{i,\mathrm{c}}^{\mathrm{X}} \tag{3.30}$$

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \frac{1}{(1-\epsilon)\rho_{\mathrm{X}}}\sum_i (J_i^{\mathrm{X}} + Lr_{i,\mathrm{c}}^{\mathrm{X}}), \quad i \neq \mathrm{ND} \tag{3.31}$$

3.3.4 Reactions – kinetics and stoichiometry

The biological reactions are modelled as taking place through a number of "processes", each process j happening at a rate ρ_j. The conversion rate r_i of a component i can then be described as $r_i = \sum_j \nu_{i,j}\rho_j$, where $\nu_{i,j}$ is the stoichiometric coefficient of the component in process j. The process rate ρ_j is controlled by Monod kinetics. The

processes and rate expressions are not identical to those defined in ASM1, but have been extended with denitrification dynamics [26] and some minor modifications to prevent negative concentrations [24]. The most important departure from ASM1 is the separation of autotrophic bacteria into AOB and NOB and the division of $NO_x{}^-$ into $NO_2{}^-$ and $NO_3{}^-$, a change that was introduced quite early in biofilm modelling for wastewater treatment [28].

The modelled phenomena with corresponding rate expressions are as follows:

1. Aerobic growth of heterotrophs

$$\rho_1 = \mu_H \frac{S_S}{K_S + S_S} \frac{S_O}{K_{O,H} + S_O} \frac{S_{NH}}{K_{NH,H} + S_{NH}} X_{BH} \tag{3.32}$$

2. Anoxic growth of heterotrophs on NO_2

$$\rho_2 = \mu_H \nu_{NO2} \frac{S_S}{K_S + S_S} \frac{K_{O,H}}{K_{O,H} + S_O} \frac{S_{NO2}}{K_{NOx} + S_{NO2}} \frac{S_{NO2}}{S_{NO2} + S_{NO3}} X_{BH} \tag{3.33}$$

3. Anoxic growth of heterotrophs on NO_3

$$\rho_3 = \mu_H \nu_{NO3} \frac{S_S}{K_S + S_S} \frac{K_{O,H}}{K_{O,H} + S_O} \frac{S_{NO3}}{K_{NOx} + S_{NO2}} \frac{S_{NO3}}{S_{NO2} + S_{NO3}} X_{BH} \tag{3.34}$$

4. Aerobic growth of AOB

$$\rho_4 = \mu_{AOB} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_O}{K_{O,A} + S_O} \frac{S_{Alk}}{K_{Alk} + S_{Alk}} X_{AOB} \tag{3.35}$$

5. Aerobic growth of NOB

$$\rho_5 = \mu_{NOB} \frac{S_{NO2}}{K_{NO2} + S_{NO2}} \frac{S_O}{K_{O,A} + S_O} \frac{S_{Alk}}{K_{Alk} + S_{Alk}} \frac{K_{NH,I}}{K_{NH,I} + S_{NH}} X_{NOB} \tag{3.36}$$

6. Decay of heterotrophs

$$\rho_6 = b_H X_{BH} \tag{3.37}$$

7. Decay of AOB

$$\rho_7 = b_{AOB} X_{AOB} \tag{3.38}$$

8. Decay of NOB

$$\rho_8 = b_{NOB} X_{NOB} \tag{3.39}$$

9. Ammonification of soluble organically bound nitrogen (S_{ND})

$$\rho_9 = k_a S_{ND} X_{BH} \tag{3.40}$$

10. Hydrolysis of particulate organic carbon (X_S)

$$\rho_{10} = k_h \frac{X_S}{K_X + X_S/X_{BH}} \left[\frac{S_O}{K_{O,H} + S_O} + \nu_h \frac{K_{O,H}}{K_{O,H} + S_O} \frac{S_{NO2} + S_{NO3}}{K_{NOx} + S_{NO2} + S_{NO3}} \right] \tag{3.41}$$

11. Hydrolysis of particulate organically bound nitrogen (X_{ND})

$$\rho_{11} = \rho_{10} \frac{X_{ND}}{X_S} \tag{3.42}$$

The stoichiometric coefficients for each component in each process are presented in Table 3.4, and the values of the various parameters that occur in the process expressions and in the stoichiometry are shown in Table 3.3. Some parameters scale with temperature according to the formula

$$p(T) = p_{20} \left(\frac{p_{20}}{p_{10}} \right)^{\frac{T-20}{10}} \tag{3.43}$$

where p_{10} and p_{20} are the parameter values at 10 and 20 °C, respectively, and T is the temperature in °C. This temperature dependency formula is valid between about 5 and 25 °C [29].

Table 3.3: Biological parameter values in the waste treatment model.

Parameter	Value at 10 °C	Value at 20 °C	Ref.	Parameter	Value	Ref.	Parameter	Value	Ref.
μ_{H}	3.0	6.0	[29]	Y_{H}	0.67	[30]	K_{S}	10.0	[30]
μ_{AOB}	0.29	0.76	[24]	Y_{AOB}	0.21	[26]	$K_{\mathrm{O,H}}$	0.2	[29]
μ_{NOB}	0.58	1.04	[24]	Y_{NOB}	0.03	[26]	$K_{\mathrm{NH,H}}$	0.01	[13]
b_{H}	0.20	0.40	[29]	ν_{NO2}	0.8	[26]	$K_{\mathrm{O,H}}$	0.2	[29]
b_{AOB}	0.05	0.15	[26]	ν_{NO3}	0.8	[26]	K_{NOx}	0.5	[29]
b_{NOB}	0.05	0.15	[26]	k_{a}	0.05	[30]	K_{NH}	1.0	[29]
k_{h}	2.0	3.0	[29]	ν_{h}	1.30	[31]	$K_{\mathrm{O,A}}$	0.5	[29]
K_{X}	0.3	0.1	[29]	i_{XB}	0.08	[30]	K_{Alk}	0.1	[29]
				i_{XP}	0.06	[30]	K_{NO2}	1.0	[27]
				f_{p}	0.08	[30]	$K_{\mathrm{NH,I}}$	5.0	[32]

Table 3.4: Bioprocess kinetics and stoichiometry. Unlisted species are not modelled in the biological reactions.

Species Process	S_I	S_S	S_O	S_{NO2}	S_{NO3}	S_{NH}	S_{ND}	S_{Alk}
1		$-\frac{1}{Y_H}$	$1-\frac{1}{Y_H}$					
2		$-\frac{1}{Y_H}$		$-\frac{1-Y_H}{1.72Y_H}$		$-i_{XB}$		$\frac{1-Y_H}{14\cdot 1.72Y_H}-\frac{i_{XB}}{14}$
3		$-\frac{1}{Y_H}$			$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$		$\frac{1-Y_H}{14\cdot 2.86Y_H}-\frac{i_{XB}}{14}$
4			$\frac{Y_{AOB}-3.43}{Y_{AOB}}$	$\frac{1}{Y_{AOB}}$		$-i_{XB}-\frac{1}{Y_{AOB}}$		$-\frac{i_{XB}}{14}-\frac{1}{7\cdot Y_{AOB}}$
5			$\frac{Y_{NOB}-1.14}{Y_{NOB}}$	$-\frac{1}{Y_{NOB}}$	$\frac{1}{Y_{NOB}}$	$-i_{XB}$		$-\frac{i_{XB}}{14}$
6								
7								
8								
9						1	-1	$\frac{1}{14}$
10		1						
11							1	

	X_I	X_S	X_{BH}	X_{AOB}	X_{NOB}	X_p	X_{ND}
1			1				
2			1				
3			1				
4				1			
5					1		
6		$1-f_p$	-1			f_p	$i_{XB}-f_p i_{XP}$
7		$1-f_p$		-1		f_p	$i_{XB}-f_p i_{XP}$
8		$1-f_p$			-1	f_p	$i_{XB}-f_p i_{XP}$
9							
10		-1					
11							-1

CHAPTER 4

Topology study

In this chapter, a study of water treatment configurations is presented [33]. It was conducted using the simulator LibRAS together with an optimization tool, and the goal was to compare the performance of some different topologies – that is, ways to arrange the treatment units – under various conditions.

Whenever things are to be compared, a very important question is *what is a just measure?* Ideally, the cases one compares should each be operating with their individual optimal control strategy. In this case, we set up the requirements of the water treatment system in the form of a TAN threshold, then used an optimization tool to find the smallest treatment volume that complied with this limit. The treatment units in the different cases are the same, only arranged differently and with different flow patterns, so biofilter volume should be a proxy for how efficient a given topology is. The optimizer also chooses how to split the flows; this is the control strategy, and by allowing it to be simultaneously optimized the comparison should be between individually optimal configurations.

The simplified culture model was used in the study, because the better computational performance was needed for the optimization. In effect, this means that we assume constant, even feeding and that fish are graded and restocked with short intervals, so that the waste production is nearly constant. A three-day average waste production is then calculated as the output from the culture model.

4.1 Topologies and cases

Three topologies were selected for comparison, along with two species of fish. Also, two different oxygenation strategies were tested: one where oxygen was supplied at 100 % saturation, and one with supersaturation to 130 %. The flow of water through the fish tank (and thus the hydraulic retention time) was adjusted to keep the effluent oxygen concentration equal; the different oxygenation strategies means that different flow rates were passed to the treatment system, causing different hydraulic retention times in the treatment units.

Furthermore, each of the in total twelve cases was tested in two variants with high and low water exchange. The high exchange was 500 $\mathrm{L/kg_{feed}}$, and the low 50 $\mathrm{L/kg_{feed}}$. This approximately corresponds to the distinction between "semi-closed" and "fully closed" RAS as given by e.g. Heldbo *et al.* [34]. In the fully closed variant, anoxic reactors for denitrification were added to prevent excessive accumulation of nitrate, and these reactors were fed with supplemental organic carbon when necessary.

To summarize, the study includes three topologies, two species of fish, two hydraulic retention times for each species, and each of these twelve cases was tested both as a semi-closed and a fully closed system.

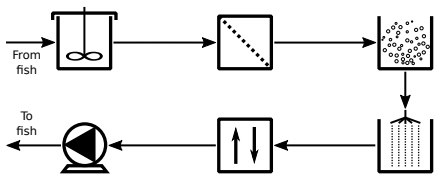
4.1.1 Topologies

The topologies in the study are illustrated in Figure 4.1, where Figure 4.1e is a legend of the symbols. The first topology (Figure 4.1a) is also the simplest possible; an inline single-pass design. The second design, shown in Figure 4.1b, has two bypass flows. This allows the residence times in the reactors to be increased, and decouples the flow through the fish tank from that through the water treatment. The third alternative uses a recycle loop (Figure 4.1c) to reduce (or possibly increase) the flow through the reactors. We will refer to these cases as "standard", "bypass" and "recycle", respectively. A more detailed description of how each topology is configured is provided below. In each configuration, all aerobic bioreactors are of equal volume, and when anoxic reactors are included, they are also of equal volume (but may differ in size from the aerobic biofilters). An example of the recycle topology is marketed by AkvaGroup (www.akvagroup.com), and several authors have written about other configurations including bypasses and/or recycling, e.g. Tal *et al.* [19] and Wik *et al.* [24].

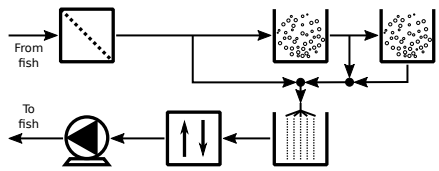
Standard

In its semi-closed variant, the standard topology begins with a particle filter which is followed by five aerated biofilters. The stream then passes through a degasser before water is exchanged.

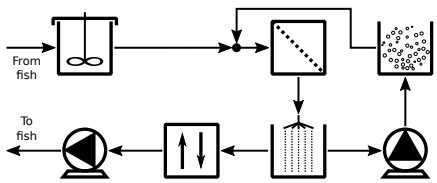
In the fully closed variant of Standard, two anoxic biofilters are added before the particle filter. The remaining topology is unaltered.



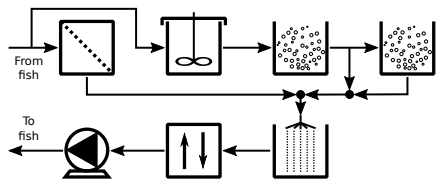
(a) Standard with optional anoxic biofilters



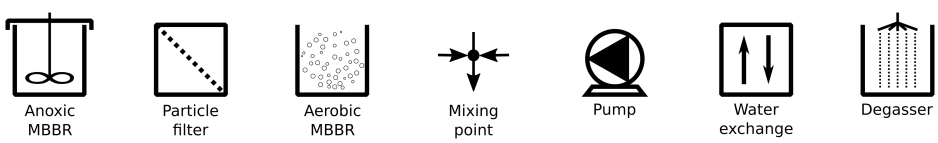
(b) Bypass without anoxic biofilters



(c) Recycle with optional anoxic biofilters



(d) Bypass with anoxic biofilters



(e) Key to symbols

Figure 4.1: The water treatment topologies compared in the study. Note that the denitrification steps (anoxic biofilters) are not included in the semi-closed cases.

Bypass

The bypass topology is slightly different in its two variants. In the semi-closed configuration (Figure 4.1b), all fish tank effluent is first passed through the particle filter. Then the flow is split in three; one branch has no biofilters, but goes directly to degassing and aeration. The "short path" has one biofilter, and the "full path" has five. The same applies to the fully closed version of the bypass topology (Figure 4.1d), but here the first split is instead made before the particle filter. The reasoning behind this was to allow particulate organic material to be available in the anoxic reactors. Again, one path has a particle filter only (no bioreactors), one path has two anoxic reactors and one aerobic, and the full treatment path has two anoxic reactors and five aerobic. Note that in the fully closed bypass configuration, the water going through biofilters does *not* pass through a particle filter!

Recycle

In the recycle topology, water from the fish tank first passes two anoxic biofilters (in the fully closed variant) and then a particle filter. It is then collected in the degassing tank, from where it is split into two branches; one goes to water exchange and back to the fish, and the other is led to five aerobic biofilters and then recycled back into the treatment stream before the particle filter. This configuration has one very important feature that sets it apart from the others: The aerobic biofilter train is fed from the degasser, and hence with already (partially) treated water. This causes a lower concentration of waste in the treatment loop than in the other configurations.

4.1.2 Fish

For the fish, we attempted to create some variation between the two cases while retaining enough similarities to simplify data collection. One case is therefore based on rainbow trout (*Oncorhynchus mykiss*) with an initial body weight of 10 g and the other is atlantic salmon (*Salmo salar*) initially at 100 g. The species were assumed to have the same body composition and eat the same feed, and were also reared at the same temperature (12 °C). Respiration rate was assumed to follow the correlation by Berg *et al.* [35], but a constant mean respiration rate was calculated for each species by averaging over the body weight of the fish.

The parameters feed conversion ratio (FCR) and thermal growth coefficient (TGC) both affect the amount of waste that is produced. The trout model has a FCR of 1.1 $\mathrm{kg_{fish}/kg_{feed}}$ and a TGC of 1.94, the same values as those used by Wik *et al.* [24] though newer research cites lower FCR values for rainbow trout ranging from 0.80 to 1.05 [36]. For salmon, the values are as recommended by Thorarensen and Farrell [7]: FCR is 0.9 $\mathrm{kg_{fish}/kg_{feed}}$ and TGC is 2.7.

Production rate

The individual fish were kept in the system for 300 days before slaughter, giving a final body weight of 0.78 kg (trout) or 3.0 kg (salmon). Every 72 h the largest fish were removed for slaughter and new small ones stocked to maintain a steady production. The total rearing volume is 11.7 m^3. With an average stocking density of 44 kg/m^3 for the salmon, this gives a monthly production rate of 130 kg and an average salmon stock of 512 kg. The rainbow trout is stocked to 60 kg/m^3, with 583 kg of fish in the system and a production rate of 170 kg per month. Table 4.2 gives a summary of the fish culture parameters.

Respiration, water flow, and retention time

For salmon, a dissolved oxygen level of 9 g/m^3 was maintained in the tanks [7]. The oxygen level required for rainbow trout is subject to some debate [37], but here we assumed a low requirement, 6 g/m^3, to contrast with the high requirement of salmon.

In the waste treatment model the fish tanks are simplified to a single mixed tank with waste addition and oxygen consumption. This simplification is valid for ideally mixed tanks connected in parallel if their hydraulic retention times are equal. The oxygen concentration in the lumped fish tank is determined by the mass of fish, their respiration rate, and the supply of oxygen provided by the incoming water. In steady state, a mass balance captures this relationship:

$$S_{\mathrm{O}} = S_{\mathrm{O,in}} - r_{\mathrm{o}}\rho\frac{V}{Q}. \tag{4.1}$$

Here, $S_{\mathrm{O,in}}$ is the inlet concentration of oxygen, ρ is the stocking density and r_{o} is the specific oxygen consumption (respiration rate), while the ratio V/Q is the hydraulic retention time. By solving this equation for the HRT, we find that the maximum retention time that will maintain an oxygen concentration of at least S_{O} in the tank at steady-state is given by

$$HRT = \frac{V}{Q} = \frac{S_{\mathrm{O,in}} - S_{\mathrm{O}}}{r_{\mathrm{o}}\rho}. \tag{4.2}$$

For salmon, Thorarensen and Farrell [7] argues that up to 120 % oxygen saturation may give better growth, but a saturation above 140 % may be detrimental to fish welfare. 130 % was therefore chosen as an intermediate level that still would give a significant reduction in water flow rate. Table 4.1 shows the flow rates and HRTs that result from maintaining the chosen oxygen concentration at these influent saturation levels.

4.1.3 Water quality

The resulting average waste production from the fish culture presented above, i.e. the sum of feed loss and fish excretions, is shown in Table 4.3. The feed loss was assumed to be 10 %.

Table 4.1: The water flows and hydraulic retention times in the four fish cases as a function of two different dissolved oxygen (DO) levels.

	Low DO	**High DO**
Influent DO [% saturation]	100	130
Influent DO [g/m^3]	10.8	14
Rainbow trout		
Fish tank DO [g/m^3]	6	6
HRT [min]	30	51
Flow rate [m^3/h]	23.4	14.0
Atlantic salmon		
Fish tank DO [g/m^3]	9	9
HRT [min]	20	56
Flow rate [m^3/h]	36.0	12.6

Table 4.2: Culture design parameters for the two fish species.

Parameter	**Salmon**	**Trout**	**Description**
IBW	100 g	10 g	Initial body weight of fish
TGC	2.7	1.94	Temperature growth coeff.
T	12 °C	12 °C	System temperature
ρ	44 kg/m^3	60 kg/m^3	Stocking density (average)
V_{tanks}	11.7 m^3	11.7 m^3	Rearing volume (total)
FCR	0.9 $\text{kg}_{\text{fish}}/\text{kg}_{\text{feed}}$	1.1 $\text{kg}_{\text{fish}}/\text{kg}_{\text{feed}}$	Feed conversion ratio
r_{o}	123 $\text{mg}/\text{kg}_{\text{fish}}$ h	190 $\text{mg}/\text{kg}_{\text{fish}}$ h	Respiration rate (oxygen consumption)
S_{O}	$\geq$9 g/m^3	$\geq$6 g/m^3	Oxygen concentration in fish tank
HRT 100 %	20 min	30 min	Hydraulic retention time
HRT 130 %	56 min	51 min	

Table 4.3: Average waste production from the simulated cultures.

	Soluble	**Particulate**
Rainbow trout		
Total ammonia nitrogen [gN/d]	168	-
Organic nitrogen [gN/d]	58	58
Biodegradable organics [gCOD/d]	1068	1381
Atlantic salmon		
Total ammonia nitrogen [gN/d]	90	-
Organic nitrogen [gN/d]	33	33
Biodegradable organics [gCOD/d]	656	853

Thorarensen and Farrell [7] compiled recommended limits for ammonia ($0.012\,\mathrm{gN/m^3}$, [38]), nitrite ($0.1\,\mathrm{gN/m^3}$, [39]) and CO_2 ($10\,\mathrm{g/m^3}$, [39]). However, as pH calculations are not yet implemented in LibRAS at the time of writing, the ammonia concentration cannot be accurately determined without further assumptions. In Terjesen *et al.* [6], a system was instead designed based on a limit on TAN, and we used the value $1\,\mathrm{gN/m^3}$ in correspondence with that paper. The nitrite limit was not enforced in the design. Nitrate was kept below $75\,\mathrm{gN/m^3}$ [14] either by water exchange (semi-closed systems) or, in the case of higher recirculation, by removal in the biological treatment.

4.2 RAS model setup

This section outlines some particularities about how the RAS model was set up in the simulator and how the model was optimized for each case.

4.2.1 Details on the water treatment model

All biofilters are modelled after the MBBR (moving bed biofilm reactor) type, implemented as two-compartment CSBRs (see Section 3.3.3 for more details) supporting $350\,\mathrm{m^2}$ of biofilm per $\mathrm{m^3}$ of bulk volume. This corresponds to e.g. 70 % filling of a carrier material with a specific area of $500\,\mathrm{m^2/m^3}$. The carriers' displacement was 18 %; in effect, one $\mathrm{m^3}$ of tank contains 126 L carrier material and 874 L of water. The aeration rate is constant and set to $k_\mathrm{L}a = 500\,\mathrm{d^{-1}}$ for the aerobic bioreactors. Anoxic bioreactors in the fully closed systems have $k_\mathrm{L}a = 0$, which means that they are assumed to be perfectly isolated from the surrounding air.

Alkalinity in the system was maintained at $2\,\mathrm{mol/m^3}$ HCO_3^--equivalents by PI control, with measurement in the last aerobic reactor and addition to the third aerobic reactor. This simulates an intent for the first two aerobic reactors to mainly consume carbon, and for reactors three to five to be nitrification tanks where alkalinity is consumed. When anoxic reactors are included in the loop, a second controller is set to dose carbon in the first anoxic tank to regulate the nitrate level at the second anoxic biofilter's output. The setpoint here is $75\,\mathrm{gN/m^3}$, and this controller must have a very gentle tuning to avoid causing instability.

The carbon dioxide stripper was modelled as a simple stirred tank with aeration ($k_\mathrm{L}a = 500\,\mathrm{d^{-1}}$) having a volume of $1.0\,\mathrm{m^3}$.

4.2.2 Optimization procedure

The remaining degrees of freedom in the treatment system – aerobic bioreactor volume, bypass/recycle ratio and, where applicable, anoxic reactor volume – were decided by optimization using a genetic algorithm [40].

A cost function was formed,

$$J = V_{\text{total}} + \alpha J_{\text{NH}} + \beta \dot{m}_{\text{COD}}, \tag{4.3}$$

which penalized total biofilter volume, added carbon (for denitrification) and violation of the TAN limit. The two tuning parameters, named α and β, were selected by careful testing. In the cost function, V_{total} is the total biofilter volume in m^3 and $\dot{m}_{\text{COD}}$ is the carbon addition (as S_{S}) in kgCOD/d. J_{NH} is a function designed to constrain the TAN concentration; the weighting α on the penalty was chosen large ($\alpha = 300$) to ensure that the limit on TAN was met. The penalty function J_{NH} was formulated as

$$J_{\text{NH}} = (S_{\text{NH}} - S_{\text{NH}}^{\max})^2 + \max(0, S_{\text{NH}} - S_{\text{NH}}^{\max}) \tag{4.4}$$

where S_{NH} is the steady-state concentration of TAN in gN/m^3 in the fish tanks and $S_{\text{NH}}^{\max} = 1\,\text{gN/m}^3$ is the concentration limit for TAN. The quadratic part of the penalty was required for the optimizer to consistently find good solutions.

The cost on carbon was chosen as $\beta = 50$. The results of the optimization are quite insensitive to this parameter as long as it is reasonably large. Its effects are discussed in more detail in Section 4.4.

The optimization software was written in Python 2.7 (Python Software Foundation, `www.python.org`) using the Pyevolve library (version 0.5, `pyevolve.sourceforge.net`). The cost function specified above resulted in a TAN concentration that for all cases were within 2 % of the target concentration $1\,\text{gN/m}^3$.

4.3 Results

All the designs maintained concentrations of dissolved carbon dioxide and nitrate below the recommended levels, but failed to keep nitrite below the maximum $0.1\,\text{g}_{\text{N}}/\text{m}^3$. Tables 4.4 and 4.5 show the numerical results for the semi-closed and fully closed systems, respectively. These results are presented with some comments below. Table 4.6 presents how the optimizer divides the flow to obtain the best treatment, while the optimized recycle rates are shown in Table 4.7.

Semi-closed configurations

In the case of the standard topology without oxygen supersaturation, the smallest treatment volume that managed the TAN limit was five reactors of $6.4\,\text{m}^3$ each for the rainbow trout. In Table 4.4, which shows the required treatment volumes for all the semi-closed cases, this case is given a normalized volume of 1. The resulting concentrations of nitrate, nitrite and soluble organics in the fish tank are also presented.

For bypass, there is no consistent pattern to the optimal flow splits. In most cases, one branch is completely shut off. The two low HRT cases for salmon are exceptions, where all three paths are used. The recycle rates also vary between cases. One should note

Table 4.4: Smallest-volume design for each semi-closed configuration that gives a TAN value of 1.0 gN/m^3. The systems contain five aerobic reactors; total reactor volume is given. Normalized values in parentheses are relative to the case Standard 100 % for Rainbow trout. Also shown are concentrations of waste components for the simulated plants in steady operation.

Case	**Volume** [m^3]	**Normalized total vol.**	**NO_3^-** [gN/m^3]	**NO_2^-** [gN/m^3]	**S_S** [g/m^3]
Rainbow trout					
Standard 100 %	32.0	**1.00** (1.00)	63	0.40	2.4
Standard 130 %	27.5	0.86 (0.86)	64	0.32	3.6
Bypass 100 %	24.5	0.77 (0.77)	60	0.19	3.3
Bypass 130 %	26.5	0.83 (0.83)	63	0.19	4.1
Recycle 100 %	46.5	1.45 (1.45)	65	0.17	5.3
Recycle 130 %	77.0	2.41 (2.41)	66	0.17	5.4
Atlantic salmon					
Standard 100 %	29.0	**1.00** (0.91)	52	0.45	1.4
Standard 130 %	18.5	0.64 (0.58)	54	0.40	2.7
Bypass 100 %	13.0	0.45 (0.41)	49	0.17	3.3
Bypass 130 %	14.0	0.48 (0.44)	51	0.16	3.6
Recycle 100 %	19.5	0.67 (0.61)	54	0.25	5.0
Recycle 130 %	26.5	0.91 (0.83)	56	0.17	6.0

Table 4.5: Smallest-volume design for each fully closed configuration that gives a TAN value of 1.0 gN/m^3. The systems contain five aerobic and two anoxic reactors; combined reactor volumes are given. Normalized volumes in parentheses are relative to the semi-closed case Standard 100 % for Rainbow trout. Waste concentrations in the simulated plants in steady operation are also shown. Nitrate is 75–76 gN/m^3.

Case	**Volume** [m^3]		**Normalized**	**Added COD**	**NO_2^-**	**S_S**
	Aerobic	Anoxic	**total vol.**	[kg/d]	[gN/m^3]	[g/m^3]
Rainbow trout						
Standard DN 100 %	29.0	16.8	**1.00** (1.43)	3.03	0.36	2.4
Standard DN 130 %	12.5	44.0	1.23 (1.77)	0.02	0.29	3.7
Bypass DN 100 %	23.0	40.0	1.38 (1.97)	0.37	0.16	5.5
Bypass DN 130 %	25.0	36.0	1.33 (1.91)	0.03	0.17	5.3
Recycle DN 100 %	9.5	3.40	0.28 (0.40)	2.41	0.13	7.1
Recycle DN 130 %	54.5	42.0	2.11 (3.02)	0.67	0.18	3.7
Atlantic salmon						
Standard DN 100 %	33.5	11.6	**1.00** (1.41)	2.08	0.43	1.3
Standard DN 130 %	9.0	48.0	1.26 (1.78)	2.65	0.36	2.7
Bypass DN 100 %	13.0	27.2	0.89 (1.26)	1.30	0.23	4.3
Bypass DN 130 %	13.5	28.0	0.92 (1.30)	0.35	0.14	6.3
Recycle DN 100 %	10.5	4.4	0.33 (0.47)	1.48	0.44	4.2
Recycle DN 130 %	5.0	3.0	0.18 (0.25)	1.29	0.09	4.9

that 10 % was set as the minimum recycle rate, because a lower flow through the branch caused numerical problems in the simulation, and already at this level the treatment units are nearly without effect.

For the recycle cases, the results are mixed. For trout, the recycle system uses more treatment volume to comply with the TAN limit. For salmon, recycle is more effective than standard in the case without supersaturated oxygen, and less effective when supersaturation is used. The bypass configuration is more volume-effective than the standard topology for all non-denitrifying systems, for both species and oxygenation strategies.

Table 4.6: Flow fractions in the different branches for the bypass configurations. The short path has two anoxic reactors (in fully closed systems only) and one aerobic, with the last four aerobic tanks bypassed.

Case	**Treatment path** [% of total flow]		
	Particle filter only	Short	Full
Rainbow trout			
Bypass 100 %	0	62	38
Bypass 130 %	0	36	64
Bypass DN 100 %	62	0	38
Bypass DN 130 %	35	0	65
Atlantic salmon			
Bypass 100 %	40	48	12
Bypass 130 %	0	63	37
Bypass DN 100 %	80	8	12
Bypass DN 130 %	63	0	37

Table 4.7: Recycle rates used in the applicable configurations. 100 % recycle rate corresponds to equal flow through aerobic reactors and fish tank. Recycle rates lower than 10 % were not investigated.

Case	**Recycle rate** [% of fish tank flow]
Rainbow trout	
Recycle 100 %	65
Recycle 130 %	180
Recycle DN 100 %	10
Recycle DN 130 %	300
Atlantic salmon	
Recycle 100 %	20
Recycle 130 %	64
Recycle DN 100 %	14
Recycle DN 130 %	10

Fully closed systems

In most cases, added denitrification reactors gave a larger total volume than the corresponding semi-closed systems. Nitrate was successfully kept at 75–76 $\mathrm{gN/m^3}$ by the

controller in all cases. Table 4.5 lists the resulting optimized volumes and waste concentrations, as well as the amount of organic carbon that is added to control the nitrate concentration, in the fully closed configurations.

4.4 Discussion

The nitrite concentration in the fish tank was in all cases above the recommended value of $0.1\,\mathrm{gN/m^3}$ [7]. However, the resulting nitrite concentration is sensitive to the model parameter μ_{NOB}, the maximum growth rate of the nitrite-oxidizing bacteria, and this parameter is subject to uncertainty. The design volume is on the other hand not sensitive to μ_{NOB}, and tuning the parameter to a higher (but still realistic) value can reduce the nitrite concentration to be below the limit. One should also note that Pedersen *et al.* [22] found higher nitrite levels acceptable for rainbow trout, and that nitrite toxicity is dependent on factors such as salinity.

Comparing the topologies, the fish tank nitrite level was lower in the two alternative configurations than in the standard case. The most important reason is likely to be dilution: Nitrite remaining after the nitrification train is mixed with non-treated (low nitrite) water before it is returned to the fish, which leads to a lower concentration in the rearing tank. Also, Wik *et al.* [24] argued that longer retention times in the nitrifying biofilters permits more nitrite to be further oxidized to nitrate.

Semi-closed systems

When increasing the oxygen content in the supply water, the required volume decreases for the standard topology while it increases for the bypass and recycle configurations. This perhaps unintuitive effect occurs because changing the HRT in the fish tank affects treatment system operation in two important but opposite directions, and which effect will dominate is dependent on the specific conditions. The first effect is that with a more concentrated oxygen supply, the flow though the fish tank is decreased, and in the standard topology the consequent increase in residence time in the biofilters makes them more efficient. The reason is that more carbon substrate is consumed early, which benefits nitrification in the later stages. This is also the probable reason for why the bypass configuration, where the biofilter residence time can be adjusted by the optimizer, is volumetrically more efficient than the standard topology.

The second and opposite effect is that because the production of waste is the same at both HRT levels, a lower flow through the fish tanks requires *better* treatment. Consider a mass balance over the fish tanks in steady state. If r_{NH} is the amount of TAN excreted by the fish ($\mathrm{g/m^3h}$) and S_{NH} is constant at $1\,\mathrm{gN/m^3}$ as required by the design, we have

that

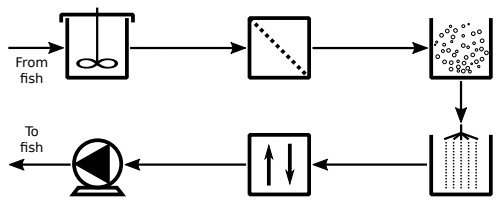
$$0 = QS_{\mathrm{NH,in}} - QS_{\mathrm{NH}} + Vr_{\mathrm{NH}} \tag{4.5}$$

$$\implies \quad S_{\mathrm{NH,in}} = S_{\mathrm{NH}} - \frac{V}{Q} r_{\mathrm{NH}}. \tag{4.6}$$

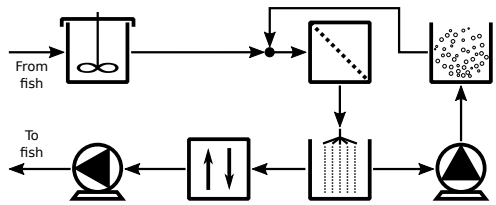
This proves that the longer the HRT (V/Q), the lower the influent concentration of TAN must be.

Additionally, there is a fundamental difference in the design of the topologies when comparing standard and bypass on the one hand to the recycle concept on the other. In the recycle topology, water is taken to treatment from the degassing tank (cf. Figure 4.2) which approximately has the concentration $S_{\mathrm{NH,in}}$ rather than S_{NH}, and since $S_{\mathrm{NH,in}} < S_{\mathrm{NH}}$, the consequent lower TAN concentration reduces the apparent nitrification rate.

The various described phenomena interact, and not one single effect is dominant in all cases. In its semi-closed variants, the recycle topology has worse volume efficiency than the standard for trout, though better than standard for salmon. Again, the balance between residence time, dilution, and required concentration in fish tank influent ($S_{\mathrm{NH,in}}$ above) cause varying effects for different conditions. The amount of organic carbon that must be processed in the aerobic section is also important, as it has an influence on the nitrification.



(a) Standard topology



(b) Recycle topology

Figure 4.2: The recycle topology has intrinsically lower concentrations in the nitrification train due to the mixing of treated and untreated streams.

Fully closed systems

Observant readers should already have noticed very low optimal volumes in some of the fully closed recycle topologies. This is because heterotrophic assimilation of TAN becomes the dominant treatment mechanism in these cases. Heterotrophic bacteria can, in an aerobic environment rich in carbon, remove TAN without creating any nitrate or nitrite. Even without supplementary carbon addition, this mechanism is significant in all the studied cases and accounts for about 42 % of the TAN removal in the "base case" of rainbow trout in Standard 100 %. When the amount of added carbon is significant, i.e. over 1 $\mathrm{kg_{COD}/d}$, it is clearly dominant. To compare, Pedersen *et al.* [22] estimated in their AQUASIM modelling study that 19–21 % of the TAN in those systems was removed by heterotrophic assimilation.

Increasing the cost β on the carbon addition in the cost function (Equation 4.3) even by a large factor ($\beta \geq 5000$) does not steer the solution to an optimum with proper denitrification. Decreasing β naturally increases the tendency for the treatment system to be based on heterotrophic assimilation. One should not consider this to be proof that denitrification is not possible in these configurations, but it suggests that it is difficult to achieve under the circumstances set in the study.

In the cases where the amount of supplementary carbon is small, denitrification does take place and successfully removes all or nearly all of the nitrogen waste. The deciding factor in whether denitrification occurs or not appears to be the mass flow of oxygen that is carried with the fish tank effluent to the anoxic tanks. Because denitrification requires anaerobic conditions, a large stream of oxygen demands lots of carbon to be consumed. With plenty of carbon and oxygen, heterotrophic assimilation becomes more significant, and in some cases all available TAN is consumed. In the cases with both low water flow rate and low DO concentration, the oxygen can be consumed by only a small (in some cases, practically insignificant) carbon addition. Most of the carbon required for the actual denitrification process is already present in the fish excretions.

Finally, particular attention should be given to the trout cases Standard DN 130 % and Bypass DN 130 %. Here, a large amount of true denitrification takes place, while the amount of supplemented carbon simultaneously is small. Salmon lacks these clear opportunities for denitrification, but in the case Bypass DN 130 % it is possible with some carbon addition.

4.4.1 Conclusions

The varying results for the different cases do not precipitate a clear winner among the configurations. What is instead clear is that the best design of the water treatment is highly dependent on the conditions imposed by the fish culture. It is reasonable to assume that the optimal residence time in the bioreactors generally is not achieved at the desired HRT in the fish tank, but with the ability to independently control the flows through biofilters and rearing tanks, better performance can be obtained.

Only in a few of the cases were any meaningful degree of denitrification reached. In those setups where too much oxygen reached the anoxic reactors, the external carbon addition led to heterotrophic assimilation of nearly all available TAN. In planning a system intended to include denitrification, careful consideration not only of the nitrogen and carbon but also the oxygen content in the fish tank effluent is required. This phenomenon is a good illustration of the complexity of RAS plants and the importance of simulations.

Finally, one should perhaps point out that while all the cases were a feasible solution was found can be considered optimal designs, they are of course only optimized with respect to the model. Aside from the issue of operating close to levels dangerous for the fish, which could be solved by introducing safety margins, there are of course significant uncertainties when modelling biological systems. The results in the study should therefore primarily be considered in a qualitative light.

CHAPTER 5

Future work

Part of the suggested future work is aimed at further developing LibRAS, but there are still a plethora of research questions that can be investigated using simulations. Looking at other fish species, reared at other temperatures and producing different waste concentrations, and the impact that has on the treatment system is one natural continuation of the topology study presented earlier. Modelling anammox treatment and comparing it to traditional nitrification and denitrification in terms of biofilter volume and energy use is another direction that could be taken, though it requires combining the ASM implementation with an anammox growth model. Control and estimation are other areas that would be interesting to look into. A few developments and further studies are, however, closer at hand:

Experimental evaluation

A natural step in any modelling work striving for completeness is to evaluate the fidelity of the model via experiments. Obtaining long enough time series of data is, due to the slow evolution of RAS in general, not feasible within the scope of this project, but roughly fitting a model to measurements from steady operation should at least give some indication of whether the parameter choices are sane or need refining.

Multi-layer biofilm discretization

As was mentioned in the description of the CSBR model, there is conceptual support for modelling transport within the biofilm by creating additional layers in the discretization, but in the version of LibRAS currently published this is not yet implemented. The

necessity of this refinement is something that should be investigated. If it is the case that a more refined model is desirable, this necessarily comes with an impact on simulation performance (time). The trade-off between refinement and computational performance is something that the user should be able to tune.

Additional rearing and feeding modes

The growth and feeding model that currently is implemented (which assumes optimal growth and optimal feeding, with complete grading at constant intervals) could be complemented by additional modes, implementing features such as

1. user-specified feeding and feed-limited growth,
2. continuous grading and re-stocking, and
3. water quality influencing fish growth rate.

More expressibility in the fish model would increase the flexibility of the simulator and give more options to the modeller.

Spatial and temporal temperature variations

The current implementations of both the fish growth and biofilm models do not explicitly include thermal dynamics. The waste treatment model does, however, have support for spatial temperature variations. This means that different parts of the modelled plant may be at different temperatures, but that the tempeature is not allowed to vary in time in the current version.

A real RAS may exhibit seasonal temperature fluctuations and the fish growth is influenced by this (reflected in the TGC model), as is the microbial growth processes in the biofilm. Support for temperature variations in time is therefore another thing that ought to make the simulator a more accurate representation of reality.

Further studies

In the topology study, both species of fish were kept at a moderate temperature (12 °C) and relatively high dissolved oxygen (6 and 9 $\mathrm{g/m^3}$). Both fish that thrive at much lower temperature (for instance Atlantic wolffish, *Anarhichas lupus*) and species that tolerate much lower DO levels (like *Clarias* spp.) are of interest to simulate and compare with the salmonids.

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APPENDIX A

Using the simulator

This appendix is intended to serve as a short introduction for users of the LibRAS software. It is not a complete manual, and at the time of writing limitations in the OpenModelica graphical interface makes it impossible to fully utilize the library without editing the code directly. The chapter is therefore more intended for readers who are interested in trying out RAS simulations than to be a reference of all functions and components in the package.

Modelica and OpenModelica

Modelica is an object-oriented language specifically designed for dynamical modelling of physical systems. Models are organized into reusable components representing physical devices or abstract submodels. The user then combines these components – for instance, resistors and capacitors or biofilters, pumps and tanks – into larger constellations, like electric circuits or water treatment systems.

Modelica code can be compiled and simulated in several different software suites, or tools. There are both commercial and free options available. One free tool is OpenModelica [25] which at the time of writing is available from `https://openmodelica.org`. LibRAS has been developed using OpenModelica 1.12, but should in principle be compatible with other Modelica simulation environments. They are, however, not tested together, which is why OpenModelica is the recommended first choice.

OMEdit is OpenModelica's graphical user interface, and is the preferred way to build models in LibRAS. OpenModelica's user manual, found on the webpage, gives a thorough

introduction to this program.

LibRAS

Obtaining the package

LibRAS is published under GNU GPL v3.0 and can be freely downloaded from GitHub (`https://github.com/FishSim/LibRAS`). Simply download the archive and unpack on your computer. No installation is required.

Loading LibRAS into OpenModelica

To load LibRAS into OMEdit's workspace, the file `package.mo` inside the LibRAS folder should be opened. Quoting from the OMEdit manual pages:

> Choose any of the following methods to open a Modelica file,
>
> - Select File > Open Model/Library File(s) from the menu.
> - Click on Open Model/Library File(s) toolbar button.
> - Click on the Open Model/Library File(s) button available at the right bottom of Welcome Perspective.
> - Press Ctrl+O.

With the package successfully loaded, it should be visible at the bottom of the left-hand *Libraries browser*. Expanding the library reveals subfolders containing all the implemented components. The 'Examples' subpackage demonstrates how components can be combined into a RAS model.

Example models

Five examples are included with LibRAS at the time of writing – a small running example of the CSBR treatment unit, a basic RAS plant, and implementations of the three topologies investigated in the thesis' simulation study.

Figure A.1 is a representation of the basic RAS model close to how it is shown in OMEdit. Starting from the top left and going anti-clockwise, the components visible are:

- The "fish tank" unit, which handles calculations of growth, feeding, and waste production. In this component the user specifies the number of rearing tanks, their volume, the maximum rearing density, the feeding regime, species of fish, composition of feed and so on.
- The particle filter. The user selects a percentage of solids that will be removed from the stream.

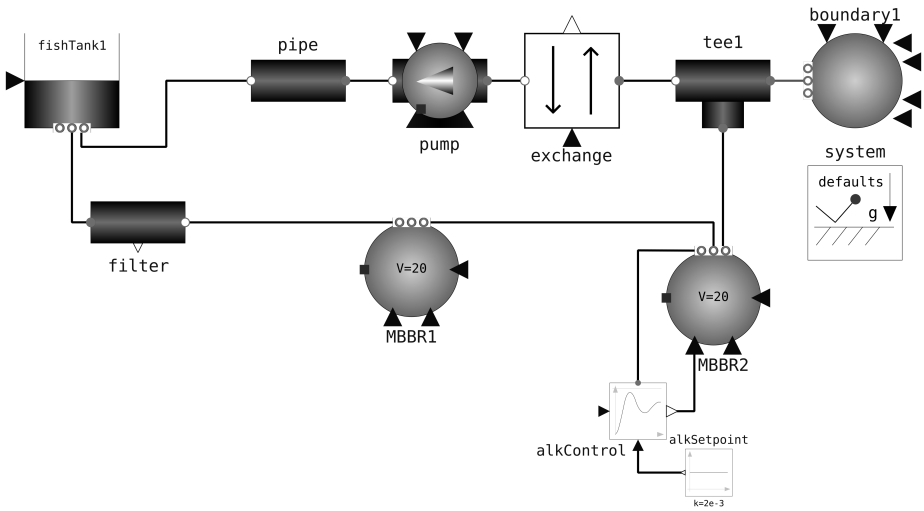

Figure A.1: The LibRAS example model "BasicRAS" as displayed in Diagram view in OMEdit.

- MBBR1, which is an aerated CSTR without any external addition of chemicals. Its volume, 20 m^3, is displayed on the component icon. Double-clicking this unit allows the user to change the volume, the $k_L a$ value and the properties of the biocarriers.
- MBBR2, identical to MBBR1 apart from it having an associated controller for alkalinity. This requires the CSBR component to have an additional *port* opened (`nPorts` = 3) as well as the flag `use_m_S_in` set to `true` to activate the external addition.
- The *System* component, which sets global parameters for the model, such as the ambient temperature, Monod parameters, and stoichiometric coefficients.
- A "boundary" component which works similarly to electrical ground, determining reference pressure and temperature. It works as a sink or source if there is flow injected or removed elsewhere in the system.
- A tee component which joins the branches. Nominally, the flow to the right is zero.
- A water exchange component which also reports how much waste is removed through this route.
- A pump which provides a set mass flow rate. The pump model is adapted from the Modelica Standard Library's Fluid package and represents a centrifugal pump.
- Finally, a pipe model – where the user can specify a height difference (static head) and/or give a pipe diameter and length for pressure drop calculations. The other components in the RAS model are without pressure drop.

The other example plants, as well as the exact models used in the topology study, have a very similar construction.

Customizing parameters

Double-clicking a component in the Diagram view will bring up the *Parameters* window. An example from the System component is shown in Figure A.2, where the user can change the biofilm parameters.

Simulating and plotting results

Pressing the green arrow starts the simulation. The default settings are to simulate for 120 days ("Stop Time") with 1 hour resolution ("Interval"). The white and green S-button in the toolbar brings up pre-simulation settings, where this may be changed. After simulation the view automatically changes to the *Plotting window*. To the right, in the *Variables browser*, all the variables in the simulation are listed and by "checking" the box next to a variable, it is plotted. In Figure A.3 an example is shown where TAN concentration (`C_S[6]`) in the fish tank (`fishTank1.fishtank`) is plotted. The components' numerical indices are translated in Table A.1. They are defined at compile time (when the user presses the simulate button) by the ordering in the files `LibRAS.Types.Species.S` and `LibRAS.Types.Species.X`.

Table A.1: Numerical indices of waste components in LibRAS for use in OMEdit's Plotting window, as defined at the time of writing.

Component	Numerical index	Description
Soluble components (S)		
I	1	inert material
S	2	biodegradable organics
O	3	dissolved oxygen
NO2	4	nitrite
NO3	5	nitrate
NH	6	total ammonia nitrogen
ND	7	organically bound nitrogen
Alk	8	alkalinity
CO2	9	dissolved carbon monoxide (NYI)
N2	10	nitrogen gas (NYI)
Particulate components (X)		
I	1	generic inert material
S	2	biodegradable organics
BH	3	heterotrophic bacteria
AOB	4	ammonia-oxidizing bacteria
NOB	5	nitrite-oxidizing bacteria
p	6	inert material from biomass decay
ND	7	organically bound nitrogen

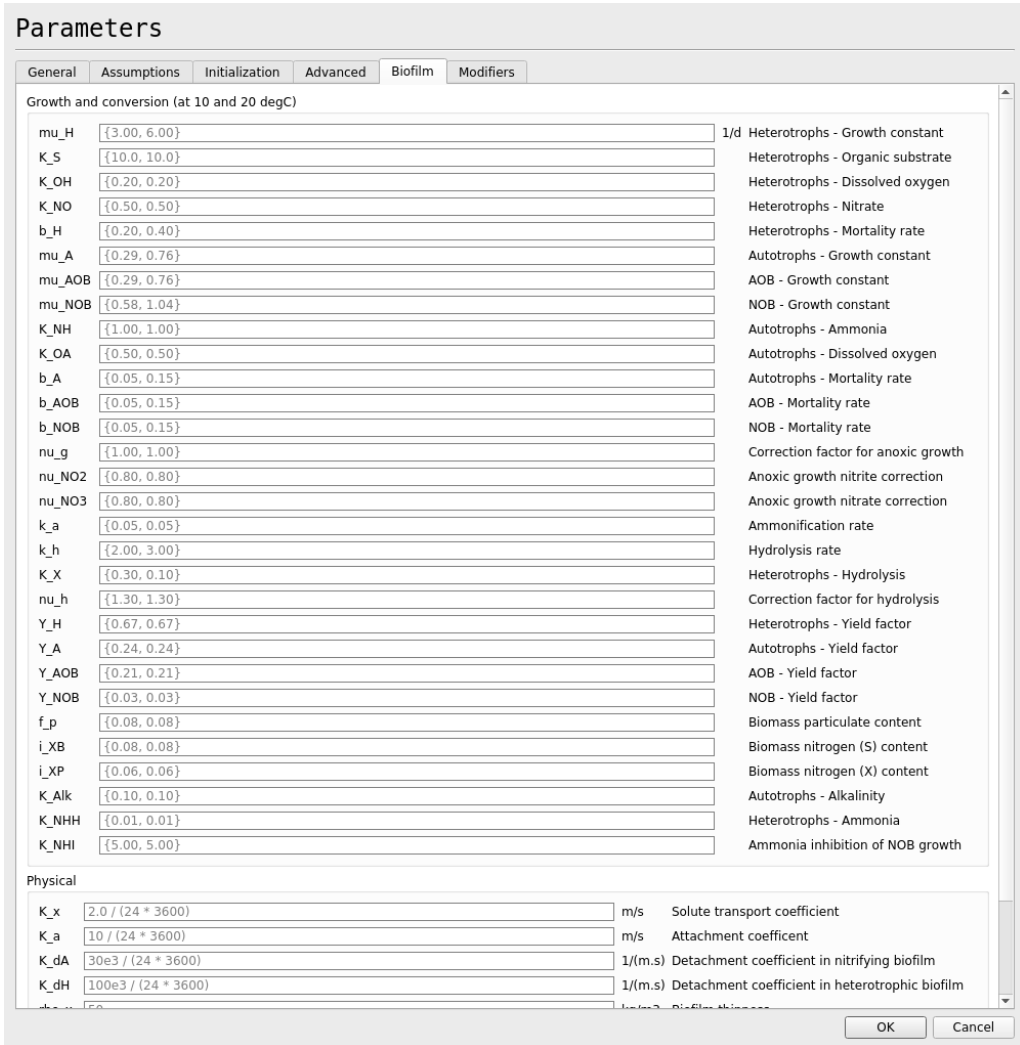

Figure A.2: Double-clicking a component brings up the parameters window. In the System component, this allows the user to set the physical biofilm parameters and parameters in the bacterial kinetics.

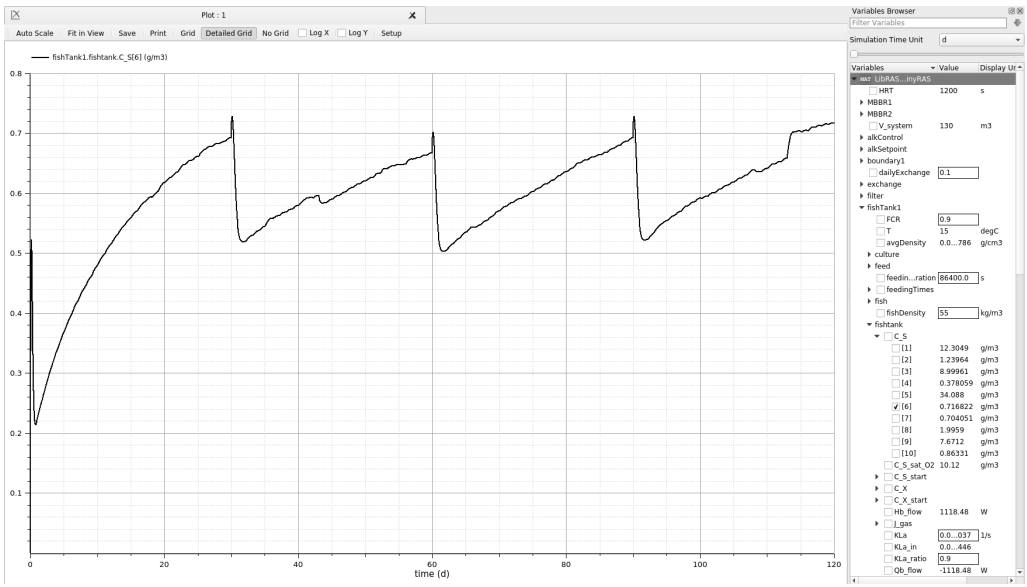

Figure A.3: OMEdit's Plotting window shows up after simulation and allows the user to browse and plot variables. Here, as an example, the TAN concentration in the fish tank is plotted over the entire simulation period.